

Fluorene-9-methanol

Other names:	(fluoren-9-yl)methanol 9-(hydroxymethyl)fluorene 9-Fluorenylmethanol 9-fluorenemethanol 9H-Fluorene-9-methanol
Inchi:	InChI=1S/C14H12O/c15-9-14-12-7-3-1-5-10(12)11-6-2-4-8-13(11)14/h1-8,14-15H,9H2
InchiKey:	XXSCONYSQQLHTH-UHFFFAOYSA-N
Formula:	C14H12O
SMILES:	OCC1c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	196.24
CAS:	24324-17-2

Physical Properties

Property code	Value	Unit	Source
gf	220.69	kJ/mol	Joback Method
hf	50.72	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Low-temperature heat capacity and standard molar enthalpy of formation of 9-fluorenemethanol (C14H12O)
hvap	68.88	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.791		Crippen Method
mcvol	155.610	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	277.30		NIST Webbook
rinpol	277.30		NIST Webbook
tb	673.42	K	Joback Method
tc	895.46	K	Joback Method
tf	411.22	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.80	J/mol×K	858.46	Joback Method
cpg	469.74	J/mol×K	895.46	Joback Method
cpg	407.08	J/mol×K	673.42	Joback Method
cpg	419.36	J/mol×K	710.43	Joback Method
cpg	430.77	J/mol×K	747.43	Joback Method
cpg	441.41	J/mol×K	784.44	Joback Method
cpg	451.39	J/mol×K	821.45	Joback Method
dvisc	0.0002303	Pa×s	673.42	Joback Method
dvisc	0.0002940	Pa×s	629.72	Joback Method
dvisc	0.0021717	Pa×s	411.22	Joback Method
dvisc	0.0012484	Pa×s	454.92	Joback Method
dvisc	0.0007908	Pa×s	498.62	Joback Method
dvisc	0.0005392	Pa×s	542.32	Joback Method
dvisc	0.0003892	Pa×s	586.02	Joback Method
hfust	26.27	kJ/mol	234.00	NIST Webbook
rhos	1084.00	kg/m ³	298.15	A combined experimental and computational thermodynamic study of fluorene-9-methanol and fluorene-9-carboxylic acid

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Low-temperature heat capacity and standard molar enthalpy of formation of fluorene-9-methanol and fluorene-9-carboxylic acid: computational thermodynamic study of fluorene-9-methanol and fluorene-9-carboxylic acid: McGowan Method:

<https://www.doi.org/10.1016/j.jct.2003.08.017>

<https://www.doi.org/10.1016/j.jct.2013.03.005>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C24324172&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhos:	Solid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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