

Phenanthrene, 1-fluoro

Inchi:	InChI=1S/C14H9F/c15-14-7-3-6-12-11-5-2-1-4-10(11)8-9-13(12)14/h1-9H
InchiKey:	CNWURRWLFUQFDT-UHFFFAOYSA-N
Formula:	C14H9F
SMILES:	Fc1cccc2c1ccc1cccc12
Mol. weight [g/mol]:	196.22

Physical Properties

Property code	Value	Unit	Source
gf	178.64	kJ/mol	Joback Method
hf	67.33	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.132		Crippen Method
mcvol	147.210	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	298.47		NIST Webbook
rinpol	298.36		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1734.00		NIST Webbook
ripol	294.92		NIST Webbook
tb	593.59	K	Joback Method
tc	835.50	K	Joback Method
tf	364.99	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.61	J/molxK	593.59	Joback Method
cpg	355.44	J/molxK	633.91	Joback Method
cpg	368.11	J/molxK	674.23	Joback Method
cpg	379.74	J/molxK	714.54	Joback Method

cpg	390.45	J/mol×K	754.86	Joback Method
cpg	400.35	J/mol×K	795.18	Joback Method
cpg	409.57	J/mol×K	835.50	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R76121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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