

Fluoranthene, 1,2,3,10b-tetrahydro-

Other names:	1,2,3,4-Tetrahydrofluoranthene 1,2,3,10b-Tetrahydrofluoranthene
Inchi:	InChI=1S/C16H14/c1-2-8-13-12(7-1)14-9-3-5-11-6-4-10-15(13)16(11)14/h1-3,5,7-9,15H,
InchiKey:	VMBZUGDYWLFLEU-UHFFFAOYSA-N
Formula:	C16H14
SMILES:	<chem>c1ccc2c(c1)-c1cccc3c1C2CCC3</chem>
Mol. weight [g/mol]:	206.28
CAS:	20279-21-4

Physical Properties

Property code	Value	Unit	Source
gf	433.18	kJ/mol	Joback Method
hf	243.34	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	57.54	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.135		Crippen Method
mcvol	167.060	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	314.60		NIST Webbook
rinpol	328.21		NIST Webbook
rinpol	316.37		NIST Webbook
rinpol	314.60		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	643.39	K	Joback Method
tc	893.80	K	Joback Method
tf	407.64	K	Joback Method
vc	0.646	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.18	J/molxK	893.80	Joback Method

cpg	507.39	J/mol×K	852.07	Joback Method
cpg	495.03	J/mol×K	810.33	Joback Method
cpg	481.89	J/mol×K	768.60	Joback Method
cpg	467.79	J/mol×K	726.86	Joback Method
cpg	452.53	J/mol×K	685.13	Joback Method
cpg	435.92	J/mol×K	643.39	Joback Method
dvisc	0.0022525	Paxs	407.64	Joback Method
dvisc	0.0014123	Paxs	643.39	Joback Method
dvisc	0.0014884	Paxs	604.10	Joback Method
dvisc	0.0015801	Paxs	564.81	Joback Method
dvisc	0.0016926	Paxs	525.52	Joback Method
dvisc	0.0018333	Paxs	486.22	Joback Method
dvisc	0.0020138	Paxs	446.93	Joback Method
hvapt	68.00	kJ/mol	434.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20279214&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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