1,2,3,4-tetrahydrofluoranthene

Other names: 1,2,3,10b-Tetrahydrofluoranthene
1,2,3,4-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: c1ccc2c(c1)-c1cccc3c1C2CCC3
Mol. weight [g/mol]: 206.28
CAS: 100652-57-1

Physical Properties

Property code	Value	Unit	Source
hfus	23.51	kJ/mol	Joback Method
ie	7.91	eV	Cheméo Relay (1.0)
log10ws	-5.76		Cheméo Relay (1.0)
logp	4.135		Crippen Method
mcvol	167.060	ml/mol	McGowan Method
tb	622.31	K	Cheméo Relay (1.0)
tf	347.15 ± 0.50	K	NIST Webbook
tf	347.20 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.92	J/mol×K	643.39	Joback Method
cpg	452.53	J/mol×K	685.13	Joback Method
cpg	467.79	J/mol×K	726.86	Joback Method
cpg	481.89	J/mol×K	768.60	Joback Method
cpg	495.03	J/mol×K	810.33	Joback Method
cpg	507.39	J/mol×K	852.07	Joback Method
cpg	519.18	J/mol×K	893.80	Joback Method
dvisc	0.0022525	Pa×s	407.64	Joback Method
dvisc	0.0020138	Pa×s	446.93	Joback Method
dvisc	0.0018333	Pa×s	486.22	Joback Method
dvisc	0.0016926	Pa×s	525.51	Joback Method

dvisc	0.0015801	Pa×s	564.81	Joback Method
dvisc	0.0014884	Pa×s	604.10	Joback Method
dvisc	0.0014123	Pa×s	643.39	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100652571&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point