

Tricyclo[8.2.2.24,7]hexadeca-4,6,10,12,13,15-hexa-5,12-dimethyl-

InChI=1S/C18H20/c1-13-11-15-3-4-16-6-8-18(14(2)12-16)10-9-17(13)7-5-15/h5-8,11-12H
InChIKey:WTRIHLSDBRSXHN-UHFFFAOYSA-N

Formula: C18H20
SMILES: Cc1cc2ccc1CCc1ccc(cc1C)CC2
Mol. weight [g/mol]: 236.35
CAS: 80548-37-4

Physical Properties

Property code	Value	Unit	Source
gf	343.34	kJ/mol	Joback Method
hf	99.31	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
ie	7.85 ± 0.05	eV	NIST Webbook
log10ws	-5.50		Crippen Method
logp	4.187		Crippen Method
mcvol	206.100	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
tb	700.20	K	Joback Method
tc	947.76	K	Joback Method
tf	414.20	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.60	J/mol×K	700.20	Joback Method
cpg	644.89	J/mol×K	906.50	Joback Method
cpg	630.65	J/mol×K	865.24	Joback Method
cpg	615.31	J/mol×K	823.98	Joback Method
cpg	598.76	J/mol×K	782.72	Joback Method
cpg	580.89	J/mol×K	741.46	Joback Method
cpg	658.12	J/mol×K	947.76	Joback Method
dvisc	0.0001998	Pa×s	700.20	Joback Method

dvisc	0.0002414	Pa×s	652.53	Joback Method
dvisc	0.0003004	Pa×s	604.87	Joback Method
dvisc	0.0003882	Pa×s	557.20	Joback Method
dvisc	0.0005262	Pa×s	509.53	Joback Method
dvisc	0.0007596	Pa×s	461.87	Joback Method
dvisc	0.0011932	Pa×s	414.20	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=C80548374&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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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