Tricyclo[10.2.2.25,8]octadeca-5,7,12,14,15,17-hexa

Other names: [3.3]Paracyclophane
[3,3']-Paracyclophane
Tricyclo[10.2.2.25,8]octadeca-5,7,12,14,15,17-hexaene
Inchi: InChI=1S/C18H20/c1-3-15-7-11-17(12-8-15)5-2-6-18-13-9-16(4-1)10-14-18/h7-14H,1-6H
InchiKey: RUVOYPXKKFOGBH-UHFFFAOYSA-N
Formula: C18H20
SMILES: c1cc2ccc1CCCc1ccc(cc1)CCC2
Mol. weight [g/mol]: 236.36

Physical Properties

Property code	Value	Unit	Source
af	0.4654		Cheméo Relay (1.0)
chs	-9967.80 ± 1.80	kJ/mol	NIST Webbook
hf	129.40 ± 3.70	kJ/mol	NIST Webbook
hfs	26.20 ± 2.60	kJ/mol	NIST Webbook
hfus	20.44	kJ/mol	Joback Method
hsub	103.20	kJ/mol	NIST Webbook
hsub	103.30 ± 1.00	kJ/mol	NIST Webbook
hvap	96.79	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-6.29		Cheméo Relay (1.0)
logp	4.351		Crippen Method
mcvol	206.100	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	646.15	K	Cheméo Relay (1.0)
tc	913.51	K	Cheméo Relay (1.0)
tf	443.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.21	J/mol×K	698.78	Joback Method
cpg	589.75	J/mol×K	742.52	Joback Method
cpg	609.45	J/mol×K	786.25	Joback Method

cpg	627.43	J/mol×K	829.99	Joback Method
cpg	643.81	J/mol×K	873.73	Joback Method
cpg	658.71	J/mol×K	917.46	Joback Method
cpg	672.26	J/mol×K	961.20	Joback Method
cps	324.30	J/mol×K	300.00	NIST Webbook
dvisc	0.0017212	Pa×s	382.12	Joback Method
dvisc	0.0008182	Pa×s	434.90	Joback Method
dvisc	0.0004569	Pa×s	487.67	Joback Method
dvisc	0.0002859	Pa×s	540.45	Joback Method
dvisc	0.0001944	Pa×s	593.23	Joback Method
dvisc	0.0001408	Pa×s	646.00	Joback Method
dvisc	0.0001071	Pa×s	698.78	Joback Method
hfust	11.76	kJ/mol	377.00	NIST Webbook
hsubt	97.80	kJ/mol	332.00	NIST Webbook
hsubt	103.00 ± 1.00	kJ/mol	332.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2913248&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
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