Simonellite

Inchi: InChI=1S/C19H24/c1-13(2)14-7-9-16-15(12-14)8-10-18-17(16)6-5-11-19(18,3)4/h7-10,12
InchiKey: XZDCNNOTTUOTGE-UHFFFAOYSA-N
Formula: C19H24
SMILES: CC(C)c1ccc2c3c(ccc2c1)C(C)(C)CCC3
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	339.99	kJ/mol	Joback Method
hf	34.30	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.577		Crippen Method
mcvol	224.490	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	348.84		NIST Webbook
rinpol	348.84		NIST Webbook
rinpol	345.79		NIST Webbook
tb	705.53	K	Joback Method
tc	943.68	K	Joback Method
tf	423.89	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.12	J/mol×K	705.53	Joback Method
cpg	654.34	J/mol×K	745.22	Joback Method
cpg	673.58	J/mol×K	784.91	Joback Method
cpg	692.06	J/mol×K	824.60	Joback Method
cpg	710.01	J/mol×K	864.30	Joback Method
cpg	727.65	J/mol×K	903.99	Joback Method
cpg	745.23	J/mol×K	943.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R278581&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume