Dehydro abietyl nitrile

Other names: [1R-(«alpha»,4a«beta»,10a«alpha»)]-1,2,3,4,4a,9,10,10a-octahydro-7-isopropyl-1,4a-dim
Inchi: InChI=1S/C20H27N/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/
InchiKey: KSODEYYYINEFHT-UHFFFAOYSA-N
Formula: C20H27N
SMILES: CC(C)c1ccc2c(c1)CCC1C(C)(C#N)CCCC21C
Mol. weight [g/mol]: 281.44
CAS: 31148-95-5

Physical Properties

Property code	Value	Unit	Source
gf	420.02	kJ/mol	Joback Method
hf	60.48	kJ/mol	Joback Method
hfus	19.35	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.344		Crippen Method
mcvol	248.560	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
tb	813.11	K	Joback Method
tc	1059.40	K	Joback Method
tf	489.01	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.24	J/mol×K	813.11	Joback Method
cpg	804.76	J/mol×K	854.16	Joback Method
cpg	827.34	J/mol×K	895.21	Joback Method
cpg	850.38	J/mol×K	936.25	Joback Method
cpg	874.23	J/mol×K	977.30	Joback Method
cpg	899.28	J/mol×K	1018.35	Joback Method
cpg	925.90	J/mol×K	1059.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31148955&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

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