octahydro-2,5,5,8a-tetramethyl-1-naphthylacetald

Inchi: InChI=1S/C16H26O/c1-12-6-7-14-15(2,3)9-5-10-16(14,4)13(12)8-11-17/h5,10-14H,6-9H2
InchiKey: HCUUTQZQMTWYDE-UHFFFAOYSA-N
Formula: C16H26O
SMILES: CC1CCC2C(C)(C)CC=CC2(C)C1CC=O
Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	53.27	kJ/mol	Joback Method
hf	-310.95	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	55.51	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.230		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
ripol	2415.00		NIST Webbook
ripol	2415.00		NIST Webbook
tb	630.33	K	Joback Method
tc	852.28	K	Joback Method
tf	369.72	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.78	J/mol×K	630.33	Joback Method
cpg	626.52	J/mol×K	667.32	Joback Method
cpg	648.07	J/mol×K	704.31	Joback Method
cpg	668.65	J/mol×K	741.31	Joback Method
cpg	688.52	J/mol×K	778.30	Joback Method
cpg	707.89	J/mol×K	815.29	Joback Method
cpg	727.02	J/mol×K	852.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R344193&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume