Ambrial

Inchi: InChI=1S/C16H26O/c1-12-6-7-14-15(2,3)9-5-10-16(14,4)13(12)8-11-17/h11,13-14H,1,5-
InchiKey: BFWKKBSHTOEBHL-UHFFFAOYSA-N
Formula: C16H26O
SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CC=O
Mol. weight [g/mol]: 234.38
CAS: 3243-36-5

Physical Properties

Property code	Value	Unit	Source
gf	84.10	kJ/mol	Joback Method
hf	-264.15	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	55.68	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.374		Crippen Method
mcvol	211.850	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1809.20		NIST Webbook
rinpol	1809.20		NIST Webbook
tb	635.00	K	Joback Method
tc	856.74	K	Joback Method
tf	386.88	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.54	J/mol×K	635.00	Joback Method
cpg	623.73	J/mol×K	671.96	Joback Method
cpg	644.80	J/mol×K	708.91	Joback Method
cpg	664.98	J/mol×K	745.87	Joback Method
cpg	684.50	J/mol×K	782.83	Joback Method
cpg	703.59	J/mol×K	819.78	Joback Method
cpg	722.49	J/mol×K	856.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3243365&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume