6-Oxo-isoambroxide

Inchi: InChI=1S/C16H26O2/c1-14(2)7-5-8-15(3)12-6-9-18-16(12,4)10-11(17)13(14)15/h12-13H
InchiKey: ZXHGUBJSXANHMV-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CC1(C)CCCC2(C)C1C(=O)CC1(C)OCCC12
Mol. weight [g/mol]: 250.38
CAS: 220766-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-22.91	kJ/mol	Joback Method
hf	-444.47	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.587		Crippen Method
mcvol	211.160	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1855.30		NIST Webbook
rinpol	1824.00		NIST Webbook
ripol	2528.00		NIST Webbook
tb	688.93	K	Joback Method
tc	940.93	K	Joback Method
tf	467.83	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.19	J/mol×K	688.93	Joback Method
cpg	682.03	J/mol×K	730.93	Joback Method
cpg	706.17	J/mol×K	772.93	Joback Method
cpg	730.10	J/mol×K	814.93	Joback Method
cpg	754.28	J/mol×K	856.93	Joback Method
cpg	779.20	J/mol×K	898.93	Joback Method

cpg	805.34	J/mol×K	940.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C220766803&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume