«beta»-Funebrene epoxide

Inchi: InChI=1S/C15H24O/c1-10-4-5-11-13(2,3)12-8-14(10,11)6-7-15(12)9-16-15/h10-12H,4-9H
InchiKey: BWDPPCMUUFETAC-HPFPLBLASA-N
Formula: C15H24O
SMILES: CC1CCC2C(C)(C)C3CC12CCC31CO1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	188.31	kJ/mol	Joback Method
hf	-194.85	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	49.25	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.628		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1586.00		NIST Webbook
ripol	2005.00		NIST Webbook
ripol	2005.00		NIST Webbook
tb	592.16	K	Joback Method
tc	829.78	K	Joback Method
tf	416.84	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.84	J/mol×K	592.16	Joback Method
cpg	564.86	J/mol×K	631.76	Joback Method
cpg	586.26	J/mol×K	671.37	Joback Method
cpg	606.55	J/mol×K	710.97	Joback Method
cpg	626.24	J/mol×K	750.57	Joback Method
cpg	645.84	J/mol×K	790.17	Joback Method
cpg	665.85	J/mol×K	829.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R397721&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume