Alloaromadendrene epoxide

Other names:	Epoxy-allo-alloaromadendrene
	Alloaromadendrene oxide
	Alloaromadendrene, epoxy
	Epoxy-allo-aromadendrene
Inchi:	InChI=1S/C15H24O/c1-9-4-5-10-12(9)13-11(14(13,2)3)6-7-15(10)8-16-15/h9-13H,4-8H2
InchiKey:	XPGWKKLDFXNBPJ-PTYHTGKGSA-N
Formula:	C15H24O
SMILES:	CC1CCC2C1C1C(CCC23CO3)C1(C)C
Mol. weight [g/mol]:	220.35
CAS:	85760-81-2

Physical Properties

Property code	Value	Unit	Source
gf	186.09	kJ/mol	Joback Method
hf	-230.43	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	50.09	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.484		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1641.00		NIST Webbook
ripol	2095.00		NIST Webbook

ripol	2095.00		NIST Webbook
ripol	2054.00		NIST Webbook
tb	587.25	K	Joback Method
tc	815.53	K	Joback Method
tf	388.70	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.52	J/mol×K	587.25	Joback Method
cpg	568.21	J/mol×K	625.30	Joback Method
cpg	590.27	J/mol×K	663.34	Joback Method
cpg	611.03	J/mol×K	701.39	Joback Method
cpg	630.84	J/mol×K	739.44	Joback Method
cpg	650.04	J/mol×K	777.48	Joback Method
cpg	668.97	J/mol×K	815.53	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85760812&Units=SI

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