trans-Anhydrolinalool oxide

Other names:	trans-Anhydrolinalool
	trans-Anhydrolinalool oxide (furanoid)
	(E)-anhydrolinalool oxide A
Inchi:	InChI=1S/C10H16O/c1-5-10(4)7-6-9(11-10)8(2)3/h5,9H,1-2,6-7H2,3-4H3/t9-,10+/m0/s1
InchiKey:	XIGFNCYVSHOLIF-VHSXEESVSA-N
Formula:	C10H16O
SMILES:	C=CC1(C)CCC(C(=C)C)O1
Mol. weight [g/mol]:	152.23
CAS:	54750-70-8

Physical Properties

Property code	Value	Unit	Source
gf	137.68	kJ/mol	Joback Method
hf	-85.28	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.686		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	993.80		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	993.80		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1254.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1253.00		NIST Webbook
ripol	1253.00		NIST Webbook
tb	459.24	K	Joback Method
tc	668.90	K	Joback Method
tf	242.11	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.19	J/mol×K	459.24	Joback Method
cpg	317.88	J/mol×K	494.18	Joback Method
cpg	334.36	J/mol×K	529.13	Joback Method
cpg	349.72	J/mol×K	564.07	Joback Method
cpg	364.10	J/mol×K	599.02	Joback Method
cpg	377.60	J/mol×K	633.96	Joback Method
cpg	390.34	J/mol×K	668.90	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54750708&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