trans-Vaccenic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C22H41NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23-22(2,3)20-24

InchiKey: YVTATXSYTQAQAB-MDZDMXLPSA-N

Formula: C22H41NO

SMILES: CCCCCCC=CCCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 335.57

Physical Properties

Property code	Value	Unit	Source
gf	296.63	kJ/mol	Joback Method
hf	-319.19	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	75.30	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.231		Crippen Method
mcvol	317.230	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2310.70		NIST Webbook
tb	807.23	K	Joback Method
tc	1001.28	K	Joback Method
tf	478.81	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.00	J/mol×K	807.23	Joback Method
cpg	1054.08	J/mol×K	839.57	Joback Method
cpg	1075.38	J/mol×K	871.91	Joback Method
cpg	1096.01	J/mol×K	904.26	Joback Method
cpg	1116.07	J/mol×K	936.60	Joback Method
cpg	1135.68	J/mol×K	968.94	Joback Method
cpg	1154.95	J/mol×K	1001.28	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=U333557&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume