Behenic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi: InChI=1S/C26H51NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27

InchiKey: OMFOMKLQJDKYOQ-UHFFFAOYSA-N

Formula: C26H51NO

SMILES: CCCCCCCCCCCCCCCCCCCCCCC1=NC(C)(C)CO1

Mol. weight [g/mol]: 393.69

Physical Properties

Property code	Value	Unit	Source
gf	250.09	kJ/mol	Joback Method
hf	-518.97	kJ/mol	Joback Method
hfus	64.68	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	9.016		Crippen Method
mcvol	377.890	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2725.60		NIST Webbook
rinpol	2725.60		NIST Webbook
tb	894.59	K	Joback Method
tc	1095.55	K	Joback Method
tf	528.97	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.57	J/mol×K	894.59	Joback Method
cpg	1340.41	J/mol×K	928.08	Joback Method
cpg	1364.43	J/mol×K	961.58	Joback Method
cpg	1387.76	J/mol×K	995.07	Joback Method
cpg	1410.52	J/mol×K	1028.56	Joback Method
cpg	1432.83	J/mol×K	1062.05	Joback Method
cpg	1454.82	J/mol×K	1095.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333109&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume