10-Methyldodec-3-en-4-olide

Inchi: InChI=1S/C13H22O2/c1-3-11(2)7-5-4-6-8-12-9-10-13(14)15-12/h9,11H,3-8,10H2,1-2H3
InchiKey: LXECKBJXFXENSF-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CCC(C)CCCCCC1=CCC(=O)O1
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-87.98	kJ/mol	Joback Method
hf	-459.50	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	54.42	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.814		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1663.00		NIST Webbook
tb	615.26	K	Joback Method
tc	817.74	K	Joback Method
tf	344.48	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.13	J/mol×K	615.26	Joback Method
cpg	517.88	J/mol×K	649.01	Joback Method
cpg	534.71	J/mol×K	682.75	Joback Method
cpg	550.65	J/mol×K	716.50	Joback Method
cpg	565.72	J/mol×K	750.25	Joback Method
cpg	579.92	J/mol×K	783.99	Joback Method
cpg	593.28	J/mol×K	817.74	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=U370412&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