10-Methyldodec-2-en-4-olide

Inchi: InChI=1S/C13H22O2/c1-3-11(2)7-5-4-6-8-12-9-10-13(14)15-12/h9-12H,3-8H2,1-2H3
InchiKey: OFMQUACVCCNBRR-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CCC(C)CCCCCC1C=CC(=O)O1
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-86.06	kJ/mol	Joback Method
hf	-468.37	kJ/mol	Joback Method
hfus	28.55	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.465		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	605.61	K	Joback Method
tc	807.05	K	Joback Method
tf	327.72	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.51	J/mol×K	605.61	Joback Method
cpg	519.92	J/mol×K	639.18	Joback Method
cpg	537.39	J/mol×K	672.76	Joback Method
cpg	553.92	J/mol×K	706.33	Joback Method
cpg	569.54	J/mol×K	739.91	Joback Method
cpg	584.26	J/mol×K	773.48	Joback Method
cpg	598.10	J/mol×K	807.05	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=U370410&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