10-Methyldodecan-5-olide

Inchi: InChI=1S/C13H24O2/c1-3-11(2)7-4-5-8-12-9-6-10-13(14)15-12/h11-12H,3-10H2,1-2H3
InchiKey: UXLFQDAATOVVOK-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CCC(C)CCCCC1CCCC(=O)O1
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-128.12	kJ/mol	Joback Method
hf	-532.31	kJ/mol	Joback Method
hfus	25.23	kJ/mol	Joback Method
hvap	53.33	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.689		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1804.00		NIST Webbook
tb	610.72	K	Joback Method
tc	816.87	K	Joback Method
tf	323.44	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.61	J/mol×K	610.72	Joback Method
cpg	544.95	J/mol×K	645.08	Joback Method
cpg	564.22	J/mol×K	679.44	Joback Method
cpg	582.45	J/mol×K	713.79	Joback Method
cpg	599.62	J/mol×K	748.15	Joback Method
cpg	615.76	J/mol×K	782.51	Joback Method
cpg	630.87	J/mol×K	816.87	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=U370408&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