10-Methylundecan-4-olide

Inchi: InChI=1S/C12H22O2/c1-10(2)6-4-3-5-7-11-8-9-12(13)14-11/h10-11H,3-9H2,1-2H3
InchiKey: ORWDJDTZZDDVQQ-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CC(C)CCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-124.44	kJ/mol	Joback Method
hf	-505.51	kJ/mol	Joback Method
hfus	24.74	kJ/mol	Joback Method
hvap	50.93	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.298		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1659.00		NIST Webbook
tb	583.57	K	Joback Method
tc	786.19	K	Joback Method
tf	315.69	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.27	J/mol×K	583.57	Joback Method
cpg	489.20	J/mol×K	617.34	Joback Method
cpg	507.19	J/mol×K	651.11	Joback Method
cpg	524.26	J/mol×K	684.88	Joback Method
cpg	540.41	J/mol×K	718.65	Joback Method
cpg	555.66	J/mol×K	752.42	Joback Method
cpg	570.01	J/mol×K	786.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370405&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