10-Methylundec-2-en-4-olide

Inchi: InChI=1S/C12H20O2/c1-10(2)6-4-3-5-7-11-8-9-12(13)14-11/h8-11H,3-7H2,1-2H3
InchiKey: MVMDDTZDLWMWNW-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(C)CCCCCC1C=CC(=O)O1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-94.48	kJ/mol	Joback Method
hf	-447.73	kJ/mol	Joback Method
hfus	25.96	kJ/mol	Joback Method
hvap	51.22	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1638.00		NIST Webbook
tb	582.73	K	Joback Method
tc	787.16	K	Joback Method
tf	316.45	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.09	J/mol×K	582.73	Joback Method
cpg	467.97	J/mol×K	616.80	Joback Method
cpg	484.95	J/mol×K	650.87	Joback Method
cpg	501.03	J/mol×K	684.94	Joback Method
cpg	516.23	J/mol×K	719.01	Joback Method
cpg	530.56	J/mol×K	753.08	Joback Method
cpg	544.04	J/mol×K	787.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370409&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

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