10-Methylundec-3-en-4-olide

Inchi: InChI=1S/C12H20O2/c1-10(2)6-4-3-5-7-11-8-9-12(13)14-11/h8,10H,3-7,9H2,1-2H3
InchiKey: YPYMVGCVXHDWKK-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(C)CCCCCC1=CCC(=O)O1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-96.40	kJ/mol	Joback Method
hf	-438.86	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.424		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1550.00		NIST Webbook
tb	592.38	K	Joback Method
tc	797.88	K	Joback Method
tf	333.21	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.83	J/mol×K	592.38	Joback Method
cpg	466.02	J/mol×K	626.63	Joback Method
cpg	482.35	J/mol×K	660.88	Joback Method
cpg	497.82	J/mol×K	695.13	Joback Method
cpg	512.45	J/mol×K	729.38	Joback Method
cpg	526.24	J/mol×K	763.63	Joback Method
cpg	539.22	J/mol×K	797.88	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=U370411&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

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