E-Dodec-5-en-4-olide

Inchi: InChI=1S/C12H20O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h7-8,11H,2-6,9-10H2,1H3/b
InchiKey: ADZMLQKJPQFTIS-BQYQJAHWSA-N
Formula: C12H20O2
SMILES: CCCCCCC=CC1CCC(=O)O1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-41.78	kJ/mol	Joback Method
hf	-383.01	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.219		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	588.17	K	Joback Method
tc	795.16	K	Joback Method
tf	325.61	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.55	J/mol×K	588.17	Joback Method
cpg	468.68	J/mol×K	622.67	Joback Method
cpg	485.86	J/mol×K	657.17	Joback Method
cpg	502.11	J/mol×K	691.66	Joback Method
cpg	517.44	J/mol×K	726.16	Joback Method
cpg	531.90	J/mol×K	760.66	Joback Method
cpg	545.49	J/mol×K	795.16	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=R412890&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