Dodec-5-yn-4-olide

Inchi: InChI=1S/C12H18O2/c1-2-3-4-5-6-7-8-11-9-10-12(13)14-11/h11H,2-6,9-10H2,1H3
InchiKey: BQEYXXKXBICFDS-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CCCCCCC#CC1CCC(=O)O1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	80.80	kJ/mol	Joback Method
hf	-227.93	kJ/mol	Joback Method
hfus	31.38	kJ/mol	Joback Method
hvap	53.47	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.666		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1714.00		NIST Webbook
tb	593.01	K	Joback Method
tc	815.58	K	Joback Method
tf	436.79	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.80	J/mol×K	593.01	Joback Method
cpg	449.95	J/mol×K	630.10	Joback Method
cpg	467.13	J/mol×K	667.20	Joback Method
cpg	483.34	J/mol×K	704.29	Joback Method
cpg	498.61	J/mol×K	741.39	Joback Method
cpg	512.92	J/mol×K	778.48	Joback Method
cpg	526.31	J/mol×K	815.58	Joback Method

Sources

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=R412954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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