(E)-Cyclanthone

Inchi: InChI=1S/C11H18O/c1-5-6-10(4)8-11(12)7-9(2)3/h5-6,9H,1,7-8H2,2-4H3/b10-6+
InchiKey: MLXAHHZSXNMVJF-UXBLZVDNSA-N
Formula: C11H18O
SMILES: C=CC=C(C)CC(=O)CC(C)C
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	69.89	kJ/mol	Joback Method
hf	-155.37	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	45.81	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.124		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1194.00		NIST Webbook
tb	505.23	K	Joback Method
tc	694.68	K	Joback Method
tf	227.86	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.66	J/mol×K	505.23	Joback Method
cpg	367.64	J/mol×K	536.80	Joback Method
cpg	381.86	J/mol×K	568.38	Joback Method
cpg	395.34	J/mol×K	599.95	Joback Method
cpg	408.13	J/mol×K	631.53	Joback Method
cpg	420.25	J/mol×K	663.10	Joback Method
cpg	431.75	J/mol×K	694.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232109&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

Latest version available from:

https://www.chemeo.com/cid/38-549-1/E-Cyclanthone.pdf

Generated by Cheméo on 2024-10-12 08:16:21.213310124 +0000 UTC m=+3301843.850279376.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.