

Cycloundecanecarboxylic acid

Inchi:	InChI=1S/C12H22O2/c13-12(14)11-9-7-5-3-1-2-4-6-8-10-11/h11H,1-10H2,(H,13,14)
InchiKey:	BHECNPOVJVTHKS-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	O=C(O)C1CCCCCCCCCCC1
Mol. weight [g/mol]:	198.30
CAS:	831-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-251.63	kJ/mol	Joback Method
hf	-532.30	kJ/mol	Joback Method
hfus	13.86	kJ/mol	Joback Method
hvap	67.02	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.602		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
tb	660.91	K	Joback Method
tc	881.05	K	Joback Method
tf	325.53	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.23	J/mol×K	660.91	Joback Method
cpg	526.34	J/mol×K	697.60	Joback Method
cpg	545.10	J/mol×K	734.29	Joback Method
cpg	562.48	J/mol×K	770.98	Joback Method
cpg	578.51	J/mol×K	807.67	Joback Method
cpg	593.16	J/mol×K	844.36	Joback Method
cpg	606.45	J/mol×K	881.05	Joback Method
dvisc	0.0197263	Pa×s	325.53	Joback Method
dvisc	0.0024902	Pa×s	381.43	Joback Method

dvisc	0.0005336	Pa×s	437.32	Joback Method
dvisc	0.0001621	Pa×s	493.22	Joback Method
dvisc	0.0000628	Pa×s	549.12	Joback Method
dvisc	0.0000290	Pa×s	605.01	Joback Method
dvisc	0.0000152	Pa×s	660.91	Joback Method

Sources

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=C831674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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