Cycloundecanecarboxylic acid, methyl ester

Other names: Methyl cycloundecanecarboxylate
Inchi: InChI=1S/C13H24O2/c1-15-13(14)12-10-8-6-4-2-3-5-7-9-11-12/h12H,2-11H2,1H3
InchiKey: WVHFSXDJALCJHN-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: COC(=O)C1CCCCCCCCCC1
Mol. weight [g/mol]: 212.33
CAS: 3667-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-211.39	kJ/mol	Joback Method
hf	-532.93	kJ/mol	Joback Method
hfus	13.55	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.690		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	614.03	K	Joback Method
tc	845.81	K	Joback Method
tf	298.21	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.12	J/mol×K	614.03	Joback Method
cpg	541.80	J/mol×K	652.66	Joback Method
cpg	564.94	J/mol×K	691.29	Joback Method
cpg	586.50	J/mol×K	729.92	Joback Method
cpg	606.46	J/mol×K	768.55	Joback Method

cpg	624.81	J/mol×K	807.18	Joback Method
cpg	641.52	J/mol×K	845.81	Joback Method
dvisc	0.0095342	Pa×s	298.21	Joback Method
dvisc	0.0020104	Pa×s	350.85	Joback Method
dvisc	0.0006363	Pa×s	403.48	Joback Method
dvisc	0.0002626	Pa×s	456.12	Joback Method
dvisc	0.0001302	Pa×s	508.76	Joback Method
dvisc	0.0000736	Pa×s	561.39	Joback Method
dvisc	0.0000459	Pa×s	614.03	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=C3667694&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume