

3-Methylenecyclobutylacetate

Inchi:	InChI=1S/C7H10O2/c1-5-3-7(4-5)9-6(2)8/h7H,1,3-4H2,2H3
InchiKey:	GECKEGSNKRNFFT-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	C=C1CC(OC(C)=O)C1
Mol. weight [g/mol]:	126.15
CAS:	18218-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-124.13	kJ/mol	Joback Method
hf	-281.73	kJ/mol	Joback Method
hfl	-484.50 ± 0.80	kJ/mol	NIST Webbook
hfus	11.55	kJ/mol	Joback Method
hvap	40.58	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.268		Crippen Method
mccvol	101.770	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	446.02	K	Joback Method
tc	646.21	K	Joback Method
tf	268.91	K	Joback Method
vc	0.385	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.45	J/mol×K	446.02	Joback Method
cpg	219.03	J/mol×K	479.38	Joback Method
cpg	230.07	J/mol×K	512.75	Joback Method
cpg	240.60	J/mol×K	546.11	Joback Method
cpg	250.61	J/mol×K	579.48	Joback Method
cpg	260.12	J/mol×K	612.84	Joback Method
cpg	269.15	J/mol×K	646.21	Joback Method
dvisc	0.0014914	Paxs	268.91	Joback Method

dvisc	0.0010778	Paxs	298.43	Joback Method
dvisc	0.0008258	Paxs	327.95	Joback Method
dvisc	0.0006612	Paxs	357.46	Joback Method
dvisc	0.0005477	Paxs	386.98	Joback Method
dvisc	0.0004659	Paxs	416.50	Joback Method
dvisc	0.0004049	Paxs	446.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18218274&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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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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