

3-Cyclopentylpropionic acid, 3-methylbut-2-yl ester

Inchi:	InChI=1S/C13H24O2/c1-10(2)11(3)15-13(14)9-8-12-6-4-5-7-12/h10-12H,4-9H2,1-3H3
InchiKey:	ZRWUBMFLUXDWDE-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	CC(C)C(C)OC(=O)CCC1CCCC1
Mol. weight [g/mol]:	212.33

Physical Properties

Property code	Value	Unit	Source
gf	-143.67	kJ/mol	Joback Method
hf	-506.53	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	53.17	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.545		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinqol	1485.00		NIST Webbook
tb	587.53	K	Joback Method
tc	785.63	K	Joback Method
tf	289.33	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.32	J/molxK	587.53	Joback Method
cpg	592.78	J/molxK	752.61	Joback Method
cpg	577.22	J/molxK	719.60	Joback Method
cpg	560.73	J/molxK	686.58	Joback Method
cpg	543.26	J/molxK	653.56	Joback Method
cpg	524.80	J/molxK	620.55	Joback Method
cpg	607.42	J/molxK	785.63	Joback Method
dvisc	0.0002063	Paxs	587.53	Joback Method
dvisc	0.0002777	Paxs	537.83	Joback Method

dvisc	0.0003971	Paxs	488.13	Joback Method
dvisc	0.0006158	Paxs	438.43	Joback Method
dvisc	0.0010684	Paxs	388.73	Joback Method
dvisc	0.0021786	Paxs	339.03	Joback Method
dvisc	0.0056744	Paxs	289.33	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=U354327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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