

Cyclohexanecarboxylic acid, 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C13H24O3/c1-11(8-9-15-2)10-16-13(14)12-6-4-3-5-7-12/h11-12H,3-10H2,1-2H
InchiKey:	GKGFDAYVMUTBPY-UHFFFAOYSA-N
Formula:	C13H24O3
SMILES:	COCCC(C)COC(=O)C1CCCCC1
Mol. weight [g/mol]:	228.33

Physical Properties

Property code	Value	Unit	Source
gf	-258.33	kJ/mol	Joback Method
hf	-639.63	kJ/mol	Joback Method
hfus	21.71	kJ/mol	Joback Method
hvap	56.14	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.783		Crippen Method
mcvol	196.480	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinsol	1646.00		NIST Webbook
tb	614.66	K	Joback Method
tc	813.47	K	Joback Method
tf	323.04	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.20	J/molxK	614.66	Joback Method
cpg	555.68	J/molxK	647.80	Joback Method
cpg	574.15	J/molxK	680.93	Joback Method
cpg	591.61	J/molxK	714.07	Joback Method
cpg	608.07	J/molxK	747.20	Joback Method
cpg	623.55	J/molxK	780.34	Joback Method
cpg	638.04	J/molxK	813.47	Joback Method
dvisc	0.0033120	Paxs	323.04	Joback Method
dvisc	0.0013664	Paxs	371.64	Joback Method

dvisc	0.0006918	Paxs	420.25	Joback Method
dvisc	0.0004034	Paxs	468.85	Joback Method
dvisc	0.0002603	Paxs	517.45	Joback Method
dvisc	0.0001811	Paxs	566.06	Joback Method
dvisc	0.0001334	Paxs	614.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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