

1,2-Cyclohexanedicarboxylic acid, butyl methyl ester

Inchi:	InChI=1S/C13H22O4/c1-3-4-9-17-13(15)11-8-6-5-7-10(11)12(14)16-2/h10-11H,3-9H2,1-
InchiKey:	ZKFODBATINMGMH-UHFFFAOYSA-N
Formula:	C13H22O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	-392.52	kJ/mol	Joback Method
hf	-767.27	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.309		Crippen Method
mvol	198.050	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	664.30	K	Joback Method
tc	866.32	K	Joback Method
tf	383.73	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.20	J/molxK	664.30	Joback Method
cpg	581.24	J/molxK	697.97	Joback Method
cpg	598.24	J/molxK	731.64	Joback Method
cpg	614.21	J/molxK	765.31	Joback Method
cpg	629.15	J/molxK	798.98	Joback Method
cpg	643.05	J/molxK	832.65	Joback Method
cpg	655.92	J/molxK	866.32	Joback Method
dvisc	0.0018145	Paxs	383.73	Joback Method

dvisc	0.0009879	Paxs	430.49	Joback Method
dvisc	0.0006059	Paxs	477.25	Joback Method
dvisc	0.0004055	Paxs	524.01	Joback Method
dvisc	0.0002899	Paxs	570.78	Joback Method
dvisc	0.0002180	Paxs	617.54	Joback Method
dvisc	0.0001707	Paxs	664.30	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339651&Units=SI

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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