

1,2-Cyclohexanedicarboxylic acid, butyl 2-methoxyethyl ester

Inchi:	InChI=1S/C15H26O5/c1-3-4-9-19-14(16)12-7-5-6-8-13(12)15(17)20-11-10-18-2/h12-13H
InchiKey:	YBGKJTGAWJQJFM-UHFFFAOYSA-N
Formula:	C15H26O5
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OCCOC
Mol. weight [g/mol]:	286.36

Physical Properties

Property code	Value	Unit	Source
gf	-480.68	kJ/mol	Joback Method
hf	-940.77	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.326		Crippen Method
mvol	232.100	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1936.00		NIST Webbook
tb	732.48	K	Joback Method
tc	929.25	K	Joback Method
tf	428.50	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.21	J/molxK	732.48	Joback Method
cpg	722.31	J/molxK	765.28	Joback Method
cpg	739.28	J/molxK	798.07	Joback Method
cpg	755.12	J/molxK	830.87	Joback Method
cpg	769.81	J/molxK	863.66	Joback Method
cpg	783.35	J/molxK	896.46	Joback Method
cpg	795.73	J/molxK	929.25	Joback Method
dvisc	0.0011258	Paxs	428.50	Joback Method
dvisc	0.0006138	Paxs	479.16	Joback Method

dvisc	0.0003758	Paxs	529.83	Joback Method
dvisc	0.0002507	Paxs	580.49	Joback Method
dvisc	0.0001785	Paxs	631.15	Joback Method
dvisc	0.0001336	Paxs	681.82	Joback Method
dvisc	0.0001041	Paxs	732.48	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=U340025&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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