

1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl ethyl ester

Inchi:	InChI=1S/C18H30O4/c1-2-21-17(19)15-10-6-7-11-16(15)18(20)22-13-12-14-8-4-3-5-9-14
InchiKey:	ILMFKDURNBJQMG-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	CCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
gf	-325.97	kJ/mol	Joback Method
hf	-816.15	kJ/mol	Joback Method
hfus	32.69	kJ/mol	Joback Method
hvap	74.52	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.870		Crippen Method
mvol	257.640	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	798.25	K	Joback Method
tc	1015.58	K	Joback Method
tf	447.46	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.52	J/molxK	798.25	Joback Method
cpg	866.22	J/molxK	834.47	Joback Method
cpg	885.24	J/molxK	870.69	Joback Method
cpg	902.61	J/molxK	906.91	Joback Method
cpg	918.35	J/molxK	943.13	Joback Method
cpg	932.48	J/molxK	979.36	Joback Method
cpg	945.01	J/molxK	1015.58	Joback Method
dvisc	0.0014280	Paxs	447.46	Joback Method

dvisc	0.0007032	Paxs	505.92	Joback Method
dvisc	0.0004011	Paxs	564.39	Joback Method
dvisc	0.0002542	Paxs	622.86	Joback Method
dvisc	0.0001742	Paxs	681.32	Joback Method
dvisc	0.0001267	Paxs	739.79	Joback Method
dvisc	0.0000966	Paxs	798.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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