

1,2-Cyclohexanedicarboxylic acid, 2-ethoxyethyl isobutyl ester

Inchi:	InChI=1S/C16H28O5/c1-4-19-9-10-20-15(17)13-7-5-6-8-14(13)16(18)21-11-12(2)3/h12-1
InchiKey:	ZCLCHKHKPBUEB-UHFFFAOYSA-N
Formula:	C16H28O5
SMILES:	CCOCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	300.39

Physical Properties

Property code	Value	Unit	Source
gf	-474.70	kJ/mol	Joback Method
hf	-966.69	kJ/mol	Joback Method
hfus	33.34	kJ/mol	Joback Method
hvap	71.66	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.572		Crippen Method
mvol	246.190	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	1956.00		NIST Webbook
tb	754.92	K	Joback Method
tc	953.14	K	Joback Method
tf	424.77	K	Joback Method
vc	0.923	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.39	J/molxK	754.92	Joback Method
cpg	780.91	J/molxK	787.96	Joback Method
cpg	798.22	J/molxK	820.99	Joback Method
cpg	814.30	J/molxK	854.03	Joback Method
cpg	829.15	J/molxK	887.07	Joback Method
cpg	842.78	J/molxK	920.11	Joback Method
cpg	855.16	J/molxK	953.14	Joback Method
dvisc	0.0012146	Paxs	424.77	Joback Method
dvisc	0.0006036	Paxs	479.79	Joback Method

dvisc	0.0003464	Paxs	534.82	Joback Method
dvisc	0.0002205	Paxs	589.85	Joback Method
dvisc	0.0001516	Paxs	644.87	Joback Method
dvisc	0.0001105	Paxs	699.89	Joback Method
dvisc	0.0000844	Paxs	754.92	Joback Method

Sources

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=U339907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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