1,2-Cyclohexanedicarboxylic acid, ethyl hexyl ester

Inchi: InChI=1S/C16H28O4/c1-3-5-6-9-12-20-16(18)14-11-8-7-10-13(14)15(17)19-4-2/h13-14H

InchiKey: DNFPNUCSOCQYSZ-UHFFFAOYSA-N

Formula: C16H28O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)OCC

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-367.26	kJ/mol	Joback Method
hf	-829.19	kJ/mol	Joback Method
hfus	35.68	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.479		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	732.94	K	Joback Method
tc	929.01	K	Joback Method
tf	417.54	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.43	J/mol×K	732.94	Joback Method
cpg	813.84	J/mol×K	896.33	Joback Method
cpg	799.62	J/mol×K	863.65	Joback Method
cpg	784.28	J/mol×K	830.97	Joback Method
cpg	767.80	J/mol×K	798.30	Joback Method
cpg	750.19	J/mol×K	765.62	Joback Method
cpg	826.93	J/mol×K	929.01	Joback Method
dvisc	0.0001198	Pa×s	732.94	Joback Method

dvisc	0.0001547	Pa×s	680.37	Joback Method
dvisc	0.0002087	Pa×s	627.81	Joback Method
dvisc	0.0002972	Pa×s	575.24	Joback Method
dvisc	0.0004546	Pa×s	522.67	Joback Method
dvisc	0.0007645	Pa×s	470.11	Joback Method
dvisc	0.0014656	Pa×s	417.54	Joback Method

Sources

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=U339406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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