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

Inchi: InChI=1S/C16H28O5/c1-3-4-7-10-20-15(17)13-8-5-6-9-14(13)16(18)21-12-11-19-2/h13-1

InchiKey: SUCFWFMYVHCNAE-UHFFFAOYSA-N

Formula: C16H28O5

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCCOC

Mol. weight [g/mol]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	-472.26	kJ/mol	Joback Method
hf	-961.41	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.716		Crippen Method
mcvol	246.190	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2041.00		NIST Webbook
rinpol	2041.00		NIST Webbook
tb	755.36	K	Joback Method
tc	951.00	K	Joback Method
tf	439.77	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.90	J/mol×K	755.36	Joback Method
cpg	841.43	J/mol×K	918.40	Joback Method
cpg	827.90	J/mol×K	885.79	Joback Method
cpg	813.17	J/mol×K	853.18	Joback Method
cpg	797.26	J/mol×K	820.57	Joback Method
cpg	780.17	J/mol×K	787.97	Joback Method
cpg	853.77	J/mol×K	951.00	Joback Method
dvisc	0.0000916	Pa×s	755.36	Joback Method

dvisc	0.0001180	Pa×s	702.76	Joback Method
dvisc	0.0001582	Pa×s	650.16	Joback Method
dvisc	0.0002236	Pa×s	597.57	Joback Method
dvisc	0.0003376	Pa×s	544.97	Joback Method
dvisc	0.0005568	Pa×s	492.37	Joback Method
dvisc	0.0010350	Pa×s	439.77	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=U340026&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