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

Inchi: InChI=1S/C20H36O5/c1-3-4-5-6-7-8-11-14-24-19(21)17-12-9-10-13-18(17)20(22)25-16-1

InchiKey: HPFXUVGIVFPCID-UHFFFAOYSA-N

Formula: C20H36O5

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

Mol. weight [g/mol]: 356.50

Physical Properties

Property code	Value	Unit	Source
gf	-438.58	kJ/mol	Joback Method
hf	-1043.97	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	80.96	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.276		Crippen Method
mcvol	302.550	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	846.88	K	Joback Method
tc	1043.91	K	Joback Method
tf	484.85	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.22	J/mol×K	846.88	Joback Method
cpg	1019.91	J/mol×K	879.72	Joback Method
cpg	1037.20	J/mol×K	912.56	Joback Method
cpg	1053.09	J/mol×K	945.40	Joback Method
cpg	1067.58	J/mol×K	978.23	Joback Method
cpg	1080.68	J/mol×K	1011.07	Joback Method
cpg	1092.41	J/mol×K	1043.91	Joback Method
dvisc	0.0007025	Pa×s	484.85	Joback Method

dvisc	0.0003600	Pa×s	545.19	Joback Method
dvisc	0.0002108	Pa×s	605.53	Joback Method
dvisc	0.0001360	Pa×s	665.87	Joback Method
dvisc	0.0000943	Pa×s	726.20	Joback Method
dvisc	0.0000692	Pa×s	786.54	Joback Method
dvisc	0.0000531	Pa×s	846.88	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=U340031&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