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

Inchi: InChI=1S/C18H32O4/c1-4-6-9-12-21-17(19)15-10-7-8-11-16(15)18(20)22-13-14(3)5-2/h1

InchiKey: LNWJBMFEEZSWPB-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)OCC(C)CC

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-352.86	kJ/mol	Joback Method
hf	-875.75	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.115		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook
tb	778.26	K	Joback Method
tc	975.02	K	Joback Method
tf	425.08	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.26	J/mol×K	778.26	Joback Method
cpg	868.53	J/mol×K	811.05	Joback Method
cpg	886.53	J/mol×K	843.85	Joback Method
cpg	903.28	J/mol×K	876.64	Joback Method
cpg	918.79	J/mol×K	909.43	Joback Method
cpg	933.07	J/mol×K	942.22	Joback Method
cpg	946.13	J/mol×K	975.02	Joback Method
dvisc	0.0014522	Pa×s	425.08	Joback Method

dvisc	0.0006791	Pa×s	483.94	Joback Method
dvisc	0.0003745	Pa×s	542.81	Joback Method
dvisc	0.0002320	Pa×s	601.67	Joback Method
dvisc	0.0001565	Pa×s	660.53	Joback Method
dvisc	0.0001127	Pa×s	719.40	Joback Method
dvisc	0.0000852	Pa×s	778.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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