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

Inchi: InChI=1S/C28H52O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-19-22-31-27(29)25-20-17-18-2

InchiKey: AGHWJGUMPFUTDW-UHFFFAOYSA-N

Formula: C28H52O4

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

Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-268.66	kJ/mol	Joback Method
hf	-1082.15	kJ/mol	Joback Method
hfus	63.23	kJ/mol	Joback Method
hvap	95.97	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	8.017		Crippen Method
mcvol	409.400	ml/mol	McGowan Method
pc	757.23	kPa	Joback Method
rinpol	3114.00		NIST Webbook
rinpol	3114.00		NIST Webbook
tb	1007.06	K	Joback Method
tc	1237.11	K	Joback Method
tf	537.78	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.18	J/mol×K	1007.06	Joback Method
cpg	1556.70	J/mol×K	1198.77	Joback Method
cpg	1544.39	J/mol×K	1160.43	Joback Method
cpg	1530.14	J/mol×K	1122.09	Joback Method
cpg	1513.90	J/mol×K	1083.74	Joback Method
cpg	1495.60	J/mol×K	1045.40	Joback Method
cpg	1567.14	J/mol×K	1237.11	Joback Method
dvisc	0.0000198	Pa×s	1007.06	Joback Method

dvisc	0.0000267	Pa×s	928.85	Joback Method
dvisc	0.0000382	Pa×s	850.63	Joback Method
dvisc	0.0000586	Pa×s	772.42	Joback Method
dvisc	0.0000990	Pa×s	694.21	Joback Method
dvisc	0.0001912	Pa×s	615.99	Joback Method
dvisc	0.0004472	Pa×s	537.78	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=U339553&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