1,2-Cyclohexanedicarboxylic acid, 3-methylbut-2-yl pentadecyl ester

Inchi: InChI=1S/C28H52O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-19-22-31-27(29)25-20-17-18-2

InchiKey: GODPKWBFJFURBF-UHFFFAOYSA-N

Formula: C28H52O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-271.10	kJ/mol	Joback Method
hf	-1087.43	kJ/mol	Joback Method
hfus	59.71	kJ/mol	Joback Method
hvap	95.58	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	8.015		Crippen Method
mcvol	409.400	ml/mol	McGowan Method
pc	760.58	kPa	Joback Method
rinpol	3067.00		NIST Webbook
rinpol	3067.00		NIST Webbook
tb	1006.62	K	Joback Method
tc	1235.49	K	Joback Method
tf	522.78	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.46	J/mol×K	1006.62	Joback Method
cpg	1495.71	J/mol×K	1044.76	Joback Method
cpg	1513.86	J/mol×K	1082.91	Joback Method
cpg	1529.96	J/mol×K	1121.05	Joback Method
cpg	1544.07	J/mol×K	1159.20	Joback Method
cpg	1556.24	J/mol×K	1197.34	Joback Method
cpg	1566.54	J/mol×K	1235.49	Joback Method
dvisc	0.0005095	Pa×s	522.78	Joback Method

dvisc	0.0002011	Pa×s	603.42	Joback Method
dvisc	0.0000989	Pa×s	684.06	Joback Method
dvisc	0.0000564	Pa×s	764.70	Joback Method
dvisc	0.0000359	Pa×s	845.34	Joback Method
dvisc	0.0000247	Pa×s	925.98	Joback Method
dvisc	0.0000180	Pa×s	1006.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339567&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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