1,2-Cyclohexanedicarboxylic acid, 2-adamantyl decyl ester

Inchi: InChI=1S/C28H46O4/c1-2-3-4-5-6-7-8-11-14-31-27(29)24-12-9-10-13-25(24)28(30)32-26
InchiKey: KPFYZJMRRSAZQH-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-111.49	kJ/mol	Joback Method
hf	-905.31	kJ/mol	Joback Method
hfus	61.20	kJ/mol	Joback Method
hvap	95.65	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.845		Crippen Method
mcvol	376.820	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	3294.00		NIST Webbook
rinpol	3294.00		NIST Webbook
tb	1022.65	K	Joback Method
tc	1252.28	K	Joback Method
tf	594.60	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1438.04	J/mol×K	1022.65	Joback Method
cpg	1458.80	J/mol×K	1060.92	Joback Method
cpg	1478.00	J/mol×K	1099.19	Joback Method
cpg	1495.75	J/mol×K	1137.47	Joback Method
cpg	1512.19	J/mol×K	1175.74	Joback Method
cpg	1527.45	J/mol×K	1214.01	Joback Method
cpg	1541.66	J/mol×K	1252.28	Joback Method
dvisc	0.0037098	Pa×s	594.60	Joback Method

dvisc	0.0027161	Pa×s	665.94	Joback Method
dvisc	0.0021122	Pa×s	737.28	Joback Method
dvisc	0.0017172	Pa×s	808.62	Joback Method
dvisc	0.0014436	Pa×s	879.97	Joback Method
dvisc	0.0012457	Pa×s	951.31	Joback Method
dvisc	0.0010972	Pa×s	1022.65	Joback Method

Sources

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=U339775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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