1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl octyl ester

Inchi: InChI=1S/C24H42O4/c1-2-3-4-5-6-12-18-27-23(25)21-15-10-11-16-22(21)24(26)28-19-1

InchiKey: ZYGQEESRISNOKD-UHFFFAOYSA-N

Formula: C24H42O4

SMILES: CCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 394.59

Physical Properties

Property code	Value	Unit	Source
gf	-275.45	kJ/mol	Joback Method
hf	-939.99	kJ/mol	Joback Method
hfus	48.23	kJ/mol	Joback Method
hvap	87.88	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.210		Crippen Method
mcvol	342.180	ml/mol	McGowan Method
pc	1072.87	kPa	Joback Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook
tb	935.53	K	Joback Method
tc	1150.78	K	Joback Method
tf	515.08	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.77	J/mol×K	935.53	Joback Method
cpg	1235.21	J/mol×K	971.41	Joback Method
cpg	1252.77	J/mol×K	1007.28	Joback Method
cpg	1268.51	J/mol×K	1043.16	Joback Method
cpg	1282.44	J/mol×K	1079.03	Joback Method
cpg	1294.61	J/mol×K	1114.91	Joback Method
cpg	1305.07	J/mol×K	1150.78	Joback Method
dvisc	0.0007366	Pa×s	515.08	Joback Method

dvisc	0.0003414	Pa×s	585.15	Joback Method
dvisc	0.0001865	Pa×s	655.23	Joback Method
dvisc	0.0001145	Pa×s	725.30	Joback Method
dvisc	0.0000766	Pa×s	795.38	Joback Method
dvisc	0.0000547	Pa×s	865.45	Joback Method
dvisc	0.0000411	Pa×s	935.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339729&Units=SI

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