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

Inchi: InChI=1S/C22H38O4/c1-2-3-4-10-16-25-21(23)19-13-8-9-14-20(19)22(24)26-17-15-18-1

InchiKey: DKUVZTYOJVMYRR-UHFFFAOYSA-N

Formula: C22H38O4

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

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-292.29	kJ/mol	Joback Method
hf	-898.71	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	83.43	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.430		Crippen Method
mcvol	314.000	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	889.77	K	Joback Method
tc	1102.80	K	Joback Method
tf	492.54	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.33	J/mol×K	889.77	Joback Method
cpg	1172.11	J/mol×K	1067.30	Joback Method
cpg	1159.18	J/mol×K	1031.79	Joback Method
cpg	1144.57	J/mol×K	996.29	Joback Method
cpg	1128.24	J/mol×K	960.78	Joback Method
cpg	1110.17	J/mol×K	925.28	Joback Method
cpg	1183.39	J/mol×K	1102.80	Joback Method
dvisc	0.0000552	Pa×s	889.77	Joback Method

dvisc	0.0000731	Pa×s	823.56	Joback Method
dvisc	0.0001018	Pa×s	757.36	Joback Method
dvisc	0.0001511	Pa×s	691.15	Joback Method
dvisc	0.0002437	Pa×s	624.95	Joback Method
dvisc	0.0004403	Pa×s	558.75	Joback Method
dvisc	0.0009325	Pa×s	492.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339727&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