cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-ethylhexyl nonyl ester

Inchi: InChI=1S/C25H44O4/c1-4-7-9-10-11-12-15-19-28-24(26)22-17-13-14-18-23(22)25(27)29
InchiKey: KULNDEAINPDFQL-UHFFFAOYSA-N
Formula: C25H44O4
SMILES: CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-263.96	kJ/mol	Joback Method
hf	-962.45	kJ/mol	Joback Method
hfus	56.68	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.622		Crippen Method
mcvol	362.830	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	2692.00		NIST Webbook
rinpol	2692.00		NIST Webbook
tb	937.58	K	Joback Method
tc	1147.94	K	Joback Method
tf	504.73	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.08	J/mol×K	937.58	Joback Method
cpg	1271.28	J/mol×K	972.64	Joback Method
cpg	1288.83	J/mol×K	1007.70	Joback Method
cpg	1304.75	J/mol×K	1042.76	Joback Method
cpg	1319.10	J/mol×K	1077.82	Joback Method
cpg	1331.90	J/mol×K	1112.88	Joback Method
cpg	1343.20	J/mol×K	1147.94	Joback Method
dvisc	0.0006508	Pa×s	504.73	Joback Method

dvisc	0.0002931	Pa×s	576.87	Joback Method
dvisc	0.0001576	Pa×s	649.01	Joback Method
dvisc	0.0000960	Pa×s	721.15	Joback Method
dvisc	0.0000639	Pa×s	793.30	Joback Method
dvisc	0.0000456	Pa×s	865.44	Joback Method
dvisc	0.0000342	Pa×s	937.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382636&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