cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-ethylbutyl octyl ester

Inchi: InChI=1S/C22H38O4/c1-4-7-8-9-10-13-16-25-21(23)19-14-11-12-15-20(19)22(24)26-17-

InchiKey: GNURDUZQURGASH-UHFFFAOYSA-N

Formula: C22H38O4

SMILES: CCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC

Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-289.22	kJ/mol	Joback Method
hf	-900.53	kJ/mol	Joback Method
hfus	48.91	kJ/mol	Joback Method
hvap	82.90	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.452		Crippen Method
mcvol	320.560	ml/mol	McGowan Method
pc	1094.99	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	868.94	K	Joback Method
tc	1069.26	K	Joback Method
tf	470.92	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.43	J/mol×K	868.94	Joback Method
cpg	1083.28	J/mol×K	902.33	Joback Method
cpg	1100.70	J/mol×K	935.71	Joback Method
cpg	1116.73	J/mol×K	969.10	Joback Method
cpg	1131.38	J/mol×K	1002.48	Joback Method
cpg	1144.69	J/mol×K	1035.87	Joback Method
cpg	1156.67	J/mol×K	1069.26	Joback Method
dvisc	0.0009203	Pa×s	470.92	Joback Method

dvisc	0.0004261	Pa×s	537.26	Joback Method
dvisc	0.0002336	Pa×s	603.59	Joback Method
dvisc	0.0001443	Pa×s	669.93	Joback Method
dvisc	0.0000972	Pa×s	736.27	Joback Method
dvisc	0.0000699	Pa×s	802.60	Joback Method
dvisc	0.0000529	Pa×s	868.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382810&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