

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

Inchi:	InChI=1S/C22H38O4/c1-4-7-9-12-16-25-21(23)19-14-10-11-15-20(19)22(24)26-17-18(6-
InchiKey:	DHMXUYLFAQOKQS-UHFFFAOYSA-N
Formula:	C22H38O4
SMILES:	CCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC
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	2395.00		NIST Webbook
rinpol	2395.00		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/molxK	868.94	Joback Method
cpg	1083.28	J/molxK	902.33	Joback Method
cpg	1100.70	J/molxK	935.71	Joback Method
cpg	1116.73	J/molxK	969.10	Joback Method
cpg	1131.38	J/molxK	1002.48	Joback Method
cpg	1144.69	J/molxK	1035.87	Joback Method
cpg	1156.67	J/molxK	1069.26	Joback Method
dvisc	0.0009203	Paxs	470.92	Joback Method

dvisc	0.0004261	Paxs	537.26	Joback Method
dvisc	0.0002336	Paxs	603.59	Joback Method
dvisc	0.0001443	Paxs	669.93	Joback Method
dvisc	0.0000972	Paxs	736.27	Joback Method
dvisc	0.0000699	Paxs	802.60	Joback Method
dvisc	0.0000529	Paxs	868.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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