

cis-Cyclohex-4-en-1,2-dicarboxylic acid, decyl 2-methylbutyl ester

Inchi:	InChI=1S/C23H40O4/c1-4-6-7-8-9-10-11-14-17-26-22(24)20-15-12-13-16-21(20)23(25)2
InchiKey:	GKAHUBCEAGNDLR-UHFFFAOYSA-N
Formula:	C23H40O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(C)CC
Mol. weight [g/mol]:	380.56

Physical Properties

Property code	Value	Unit	Source
gf	-280.80	kJ/mol	Joback Method
hf	-921.17	kJ/mol	Joback Method
hfus	51.50	kJ/mol	Joback Method
hvap	85.13	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.842		Crippen Method
mcvol	334.650	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	891.82	K	Joback Method
tc	1094.61	K	Joback Method
tf	482.19	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.49	J/molxK	891.82	Joback Method
cpg	1145.43	J/molxK	925.62	Joback Method
cpg	1162.89	J/molxK	959.42	Joback Method
cpg	1178.89	J/molxK	993.22	Joback Method
cpg	1193.46	J/molxK	1027.01	Joback Method
cpg	1206.62	J/molxK	1060.81	Joback Method
cpg	1218.41	J/molxK	1094.61	Joback Method
dvisc	0.0008228	Paxs	482.19	Joback Method

dvisc	0.0003773	Paxs	550.46	Joback Method
dvisc	0.0002055	Paxs	618.73	Joback Method
dvisc	0.0001263	Paxs	687.00	Joback Method
dvisc	0.0000847	Paxs	755.28	Joback Method
dvisc	0.0000608	Paxs	823.55	Joback Method
dvisc	0.0000458	Paxs	891.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382696&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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