

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

Inchi:	InChI=1S/C24H42O4/c1-3-5-7-9-10-11-12-16-20-28-24(26)22-18-14-13-17-21(22)23(25)
InchiKey:	QAFVJDYSTTZYKR-UHFFFAOYSA-N
Formula:	C24H42O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC
Mol. weight [g/mol]:	394.59

Physical Properties

Property code	Value	Unit	Source
gf	-269.94	kJ/mol	Joback Method
hf	-936.53	kJ/mol	Joback Method
hfus	57.62	kJ/mol	Joback Method
hvap	87.74	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.376		Crippen Method
mvol	348.740	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	915.14	K	Joback Method
tc	1120.90	K	Joback Method
tf	508.46	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.64	J/molxK	915.14	Joback Method
cpg	1207.70	J/molxK	949.43	Joback Method
cpg	1225.21	J/molxK	983.73	Joback Method
cpg	1241.20	J/molxK	1018.02	Joback Method
cpg	1255.71	J/molxK	1052.31	Joback Method
cpg	1268.77	J/molxK	1086.61	Joback Method
cpg	1280.40	J/molxK	1120.90	Joback Method
dvisc	0.0006454	Paxs	508.46	Joback Method

dvisc	0.0003160	Paxs	576.24	Joback Method
dvisc	0.0001798	Paxs	644.02	Joback Method
dvisc	0.0001139	Paxs	711.80	Joback Method
dvisc	0.0000781	Paxs	779.58	Joback Method
dvisc	0.0000569	Paxs	847.36	Joback Method
dvisc	0.0000434	Paxs	915.14	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382667&Units=SI

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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