

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

Inchi:	InChI=1S/C24H42O4/c1-4-5-6-7-8-9-10-13-18-27-23(25)21-16-11-12-17-22(21)24(26)28
InchiKey:	XMCMJELDIRPLHH-UHFFFAOYSA-N
Formula:	C24H42O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	394.59

Physical Properties

Property code	Value	Unit	Source
gf	-272.38	kJ/mol	Joback Method
hf	-941.81	kJ/mol	Joback Method
hfus	54.09	kJ/mol	Joback Method
hvap	87.35	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.232		Crippen Method
mvol	348.740	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2646.00		NIST Webbook
tb	914.70	K	Joback Method
tc	1120.82	K	Joback Method
tf	493.46	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.06	J/molxK	914.70	Joback Method
cpg	1269.05	J/molxK	1086.47	Joback Method
cpg	1256.05	J/molxK	1052.11	Joback Method
cpg	1241.59	J/molxK	1017.76	Joback Method
cpg	1225.62	J/molxK	983.41	Joback Method
cpg	1208.12	J/molxK	949.05	Joback Method
cpg	1280.61	J/molxK	1120.82	Joback Method
dvisc	0.0000397	Paxs	914.70	Joback Method
dvisc	0.0000527	Paxs	844.49	Joback Method

dvisc	0.0000737	Paxs	774.29	Joback Method
dvisc	0.0001102	Paxs	704.08	Joback Method
dvisc	0.0001802	Paxs	633.87	Joback Method
dvisc	0.0003330	Paxs	563.67	Joback Method
dvisc	0.0007330	Paxs	493.46	Joback Method

Sources

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=U382675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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