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

Inchi: InChI=1S/C24H42O4/c1-4-7-8-9-10-11-12-15-18-27-23(25)21-16-13-14-17-22(21)24(26)
InchiKey: VCYVWAOHWVAIMS-UHFFFAOYSA-N
Formula: C24H42O4
SMILES: CCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
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
mcvol	348.740	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	914.70	K	Joback Method
tc	1120.82	K	Joback Method
tf	493.46	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.06	J/mol×K	914.70	Joback Method
cpg	1269.05	J/mol×K	1086.47	Joback Method
cpg	1256.05	J/mol×K	1052.11	Joback Method
cpg	1241.59	J/mol×K	1017.76	Joback Method
cpg	1225.62	J/mol×K	983.41	Joback Method
cpg	1208.12	J/mol×K	949.05	Joback Method
cpg	1280.61	J/mol×K	1120.82	Joback Method
dvisc	0.0000397	Pa×s	914.70	Joback Method

dvisc	0.0000527	Pa×s	844.49	Joback Method
dvisc	0.0000737	Pa×s	774.29	Joback Method
dvisc	0.0001102	Pa×s	704.08	Joback Method
dvisc	0.0001802	Pa×s	633.87	Joback Method
dvisc	0.0003330	Pa×s	563.67	Joback Method
dvisc	0.0007330	Pa×s	493.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382812&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

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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