

cis-Cyclohex-4-en-1,2-dicarboxylic acid, heptyl tridecyl ester

Inchi:	InChI=1S/C28H50O4/c1-3-5-7-9-10-11-12-13-14-16-20-24-32-28(30)26-22-18-17-21-25(
InchiKey:	ILNHVAYEBKHFKK-UHFFFAOYSA-N
Formula:	C28H50O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCC
Mol. weight [g/mol]:	450.69

Physical Properties

Property code	Value	Unit	Source
gf	-236.26	kJ/mol	Joback Method
hf	-1019.09	kJ/mol	Joback Method
hfus	67.98	kJ/mol	Joback Method
hvap	96.65	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.937		Crippen Method
mvol	405.100	ml/mol	McGowan Method
pc	769.04	kPa	Joback Method
rinpol	3088.00		NIST Webbook
tb	1006.66	K	Joback Method
tc	1237.24	K	Joback Method
tf	553.54	K	Joback Method
vc	1.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1443.01	J/molxK	1006.66	Joback Method
cpg	1522.92	J/molxK	1198.81	Joback Method
cpg	1510.76	J/molxK	1160.38	Joback Method
cpg	1496.76	J/molxK	1121.95	Joback Method
cpg	1480.83	J/molxK	1083.52	Joback Method
cpg	1462.94	J/molxK	1045.09	Joback Method
cpg	1533.29	J/molxK	1237.24	Joback Method
dvisc	0.0000239	Paxs	1006.66	Joback Method
dvisc	0.0000317	Paxs	931.14	Joback Method

dvisc	0.0000440	Paxs	855.62	Joback Method
dvisc	0.0000651	Paxs	780.10	Joback Method
dvisc	0.0001047	Paxs	704.58	Joback Method
dvisc	0.0001889	Paxs	629.06	Joback Method
dvisc	0.0004005	Paxs	553.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382689&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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