

cis-Cyclohex-4-en-1,2-dicarboxylic acid, isoheptyl octadecyl ester

Inchi:	InChI=1S/C32H58O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-26-35-31(33)29-24
InchiKey:	NNNUUHJTWVWLCP-UHFFFAOYSA-N
Formula:	C32H58O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	506.80

Physical Properties

Property code	Value	Unit	Source
gf	-205.02	kJ/mol	Joback Method
hf	-1106.93	kJ/mol	Joback Method
hfus	74.81	kJ/mol	Joback Method
hvap	105.16	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	9.353		Crippen Method
mcvol	461.460	ml/mol	McGowan Method
pc	630.66	kPa	Joback Method
rinpol	3451.00		NIST Webbook
rinpol	3451.00		NIST Webbook
tb	1097.74	K	Joback Method
tc	1369.98	K	Joback Method
tf	583.62	K	Joback Method
vc	1.788	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1701.51	J/molxK	1097.74	Joback Method
cpg	1778.46	J/molxK	1324.61	Joback Method
cpg	1768.28	J/molxK	1279.23	Joback Method
cpg	1755.63	J/molxK	1233.86	Joback Method
cpg	1740.37	J/molxK	1188.49	Joback Method
cpg	1722.37	J/molxK	1143.11	Joback Method
cpg	1786.28	J/molxK	1369.98	Joback Method
dvisc	0.0000116	Paxs	1097.74	Joback Method

dvisc	0.0000157	Paxs	1012.05	Joback Method
dvisc	0.0000224	Paxs	926.37	Joback Method
dvisc	0.0000343	Paxs	840.68	Joback Method
dvisc	0.0000579	Paxs	754.99	Joback Method
dvisc	0.0001118	Paxs	669.31	Joback Method
dvisc	0.0002618	Paxs	583.62	Joback Method

Sources

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=U382749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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