

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

Inchi:	InChI=1S/C31H56O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-34-30(32)28-23-
InchiKey:	CEJQKBPYFOWEKI-UHFFFAOYSA-N
Formula:	C31H56O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
Mol. weight [g/mol]:	492.77

Physical Properties

Property code	Value	Unit	Source
gf	-213.44	kJ/mol	Joback Method
hf	-1086.29	kJ/mol	Joback Method
hfus	72.22	kJ/mol	Joback Method
hvap	102.94	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.963		Crippen Method
mcvol	447.370	ml/mol	McGowan Method
pc	662.21	kPa	Joback Method
rinpol	3347.00		NIST Webbook
tb	1074.86	K	Joback Method
tc	1334.18	K	Joback Method
tf	572.35	K	Joback Method
vc	1.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.73	J/molxK	1074.86	Joback Method
cpg	1657.29	J/molxK	1118.08	Joback Method
cpg	1675.23	J/molxK	1161.30	Joback Method
cpg	1690.68	J/molxK	1204.52	Joback Method
cpg	1703.72	J/molxK	1247.74	Joback Method
cpg	1714.47	J/molxK	1290.96	Joback Method
cpg	1723.04	J/molxK	1334.18	Joback Method
dvisc	0.0003004	Paxs	572.35	Joback Method
dvisc	0.0001291	Paxs	656.10	Joback Method

dvisc	0.0000672	Paxs	739.85	Joback Method
dvisc	0.0000400	Paxs	823.61	Joback Method
dvisc	0.0000261	Paxs	907.36	Joback Method
dvisc	0.0000184	Paxs	991.11	Joback Method
dvisc	0.0000136	Paxs	1074.86	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=U382819&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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