

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

Inchi:	InChI=1S/C29H52O4/c1-3-5-7-9-11-12-13-14-15-17-21-25-33-29(31)27-23-19-18-22-26(
InchiKey:	NRVJQGMHMDDTNI-UHFFFAOYSA-N
Formula:	C29H52O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCCC
Mol. weight [g/mol]:	464.72

Physical Properties

Property code	Value	Unit	Source
gf	-227.84	kJ/mol	Joback Method
hf	-1039.73	kJ/mol	Joback Method
hfus	70.57	kJ/mol	Joback Method
hvap	98.87	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.327		Crippen Method
mcvol	419.190	ml/mol	McGowan Method
pc	729.67	kPa	Joback Method
rinpol	3172.00		NIST Webbook
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tb	1029.54	K	Joback Method
tc	1269.23	K	Joback Method
tf	564.81	K	Joback Method
vc	1.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.35	J/molxK	1029.54	Joback Method
cpg	1527.56	J/molxK	1069.49	Joback Method
cpg	1545.56	J/molxK	1109.44	Joback Method
cpg	1561.43	J/molxK	1149.39	Joback Method
cpg	1575.24	J/molxK	1189.34	Joback Method
cpg	1587.06	J/molxK	1229.28	Joback Method
cpg	1596.97	J/molxK	1269.23	Joback Method
dvisc	0.0003529	Paxs	564.81	Joback Method

dvisc	0.0001651	Paxs	642.26	Joback Method
dvisc	0.0000909	Paxs	719.72	Joback Method
dvisc	0.0000563	Paxs	797.17	Joback Method
dvisc	0.0000379	Paxs	874.63	Joback Method
dvisc	0.0000272	Paxs	952.08	Joback Method
dvisc	0.0000205	Paxs	1029.54	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=U382690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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