

1,2-Cyclohexanedicarboxylic acid, methyl octadecyl ester

Inchi:	InChI=1S/C27H50O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-31-27(29)25-22-
InchiKey:	JKFILNSENDUOAZ-UHFFFAOYSA-N
Formula:	C27H50O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	438.68

Physical Properties

Property code	Value	Unit	Source
gf	-274.64	kJ/mol	Joback Method
hf	-1056.23	kJ/mol	Joback Method
hfus	64.17	kJ/mol	Joback Method
hvap	94.13	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.771		Crippen Method
mvol	395.310	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	3150.00		NIST Webbook
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tb	984.62	K	Joback Method
tc	1207.94	K	Joback Method
tf	541.51	K	Joback Method
vc	1.528	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.41	J/molxK	984.62	Joback Method
cpg	1492.98	J/molxK	1170.72	Joback Method
cpg	1480.19	J/molxK	1133.50	Joback Method
cpg	1465.59	J/molxK	1096.28	Joback Method
cpg	1449.13	J/molxK	1059.06	Joback Method
cpg	1430.75	J/molxK	1021.84	Joback Method
cpg	1504.00	J/molxK	1207.94	Joback Method
dvisc	0.0000254	Paxs	984.62	Joback Method

dvisc	0.0000338	Paxs	910.77	Joback Method
dvisc	0.0000473	Paxs	836.92	Joback Method
dvisc	0.0000706	Paxs	763.07	Joback Method
dvisc	0.0001148	Paxs	689.21	Joback Method
dvisc	0.0002099	Paxs	615.36	Joback Method
dvisc	0.0004525	Paxs	541.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339664&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
h_{vap}:	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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