

1,2-Cyclohexanedicarboxylic acid, ethyl 4-octyl ester

Inchi:	InChI=1S/C18H32O4/c1-4-7-11-14(10-5-2)22-18(20)16-13-9-8-12-15(16)17(19)21-6-3/h
InchiKey:	NJBGOKSKMMCTPP-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	CCCCC(CCC)OC(=O)C1CCCCC1C(=O)OCC
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-352.86	kJ/mol	Joback Method
hf	-875.75	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.258		Crippen Method
mvol	268.500	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	778.26	K	Joback Method
tc	975.02	K	Joback Method
tf	425.08	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.26	J/molxK	778.26	Joback Method
cpg	868.53	J/molxK	811.05	Joback Method
cpg	886.53	J/molxK	843.85	Joback Method
cpg	903.28	J/molxK	876.64	Joback Method
cpg	918.79	J/molxK	909.43	Joback Method
cpg	933.07	J/molxK	942.22	Joback Method
cpg	946.13	J/molxK	975.02	Joback Method
dvisc	0.0014522	Paxs	425.08	Joback Method

dvisc	0.0006791	Paxs	483.94	Joback Method
dvisc	0.0003745	Paxs	542.81	Joback Method
dvisc	0.0002320	Paxs	601.67	Joback Method
dvisc	0.0001565	Paxs	660.53	Joback Method
dvisc	0.0001127	Paxs	719.40	Joback Method
dvisc	0.0000852	Paxs	778.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339516&Units=SI

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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