

Hexanedioic acid, dicyclohexyl ester

Other names:	Adipic acid, dicyclohexyl ester Dicyclohexyl adipate Ergoplast ADC Sipalin AOC Dicyclohexyl hexanedioate
Inchi:	InChI=1S/C18H30O4/c19-17(21-15-9-3-1-4-10-15)13-7-8-14-18(20)22-16-11-5-2-6-12-16
InchiKey:	UTGUHFOMNVLJSL-UHFFFAOYSA-N
Formula:	C18H30O4
SMILES:	O=C(CCCCC(=O)OC1CCCCC1)OC1CCCCC1
Mol. weight [g/mol]:	310.43
CAS:	849-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-318.26	kJ/mol	Joback Method
hf	-795.81	kJ/mol	Joback Method
hfus	31.62	kJ/mol	Joback Method
hvap	106.30 ± 1.50	kJ/mol	NIST Webbook
log10ws	-5.10		Crippen Method
logp	4.299		Crippen Method
mcvol	257.640	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2282.00		NIST Webbook
rinpol	2247.00		NIST Webbook
rinpol	2254.00		NIST Webbook
rinpol	2261.00		NIST Webbook
rinpol	2269.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	802.92	K	Joback Method
tc	1020.34	K	Joback Method
tf	308.50 ± 1.00	K	NIST Webbook
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.49	J/molxK	802.92	Joback Method
cpg	862.70	J/molxK	839.16	Joback Method
cpg	881.29	J/molxK	875.39	Joback Method
cpg	898.28	J/molxK	911.63	Joback Method
cpg	913.69	J/molxK	947.87	Joback Method
cpg	927.55	J/molxK	984.11	Joback Method
cpg	939.90	J/molxK	1020.34	Joback Method
dvisc	0.0013745	Paxs	451.70	Joback Method
dvisc	0.0006431	Paxs	510.24	Joback Method
dvisc	0.0003518	Paxs	568.77	Joback Method
dvisc	0.0002154	Paxs	627.31	Joback Method
dvisc	0.0001434	Paxs	685.85	Joback Method
dvisc	0.0001018	Paxs	744.38	Joback Method
dvisc	0.0000759	Paxs	802.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C849990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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