

1,2-Cyclohexanedicarboxylic acid, allyl octyl ester

Inchi:	InChI=1S/C19H32O4/c1-3-5-6-7-8-11-15-23-19(21)17-13-10-9-12-16(17)18(20)22-14-4-2
InchiKey:	UGIAXNQLOZWTFN-UHFFFAOYSA-N
Formula:	C19H32O4
SMILES:	C=CCOC(=O)C1CCCCC1C(=O)OCCCCCCCC
Mol. weight [g/mol]:	324.45

Physical Properties

Property code	Value	Unit	Source
gf	-254.16	kJ/mol	Joback Method
hf	-765.68	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	75.65	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.426		Crippen Method
mvol	278.290	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	798.26	K	Joback Method
tc	994.54	K	Joback Method
tf	449.59	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.01	J/molxK	798.26	Joback Method
cpg	963.19	J/molxK	961.82	Joback Method
cpg	949.39	J/molxK	929.11	Joback Method
cpg	934.38	J/molxK	896.40	Joback Method
cpg	918.17	J/molxK	863.69	Joback Method
cpg	900.72	J/molxK	830.97	Joback Method
cpg	975.82	J/molxK	994.54	Joback Method
dvisc	0.0000863	Paxs	798.26	Joback Method

dvisc	0.0001120	Paxs	740.15	Joback Method
dvisc	0.0001519	Paxs	682.04	Joback Method
dvisc	0.0002181	Paxs	623.92	Joback Method
dvisc	0.0003372	Paxs	565.81	Joback Method
dvisc	0.0005761	Paxs	507.70	Joback Method
dvisc	0.0011304	Paxs	449.59	Joback Method

Sources

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=U339486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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