

Adipic acid, di(8-chlorooctyl) ester

Inchi: InChI=1S/C22H40Cl2O4/c23-17-11-5-1-3-7-13-19-27-21(25)15-9-10-16-22(26)28-20-14-
InchiKey: JSYHJQNEMOYMQH-UHFFFAOYSA-N
Formula: C22H40Cl2O4
SMILES: O=C(CCCCC(=O)OCCCCCCCCCl)OCCCCCCCCCl
Mol. weight [g/mol]: 439.46

Physical Properties

Property code	Value	Unit	Source
gf	-357.34	kJ/mol	Joback Method
hf	-1018.49	kJ/mol	Joback Method
hfus	66.70	kJ/mol	Joback Method
hvap	91.65	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.792		Crippen Method
mvol	360.200	ml/mol	McGowan Method
pc	911.63	kPa	Joback Method
rinpol	3193.00		NIST Webbook
rinpol	3193.00		NIST Webbook
tb	930.20	K	Joback Method
tc	1139.78	K	Joback Method
tf	541.86	K	Joback Method
vc	1.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.63	J/molxK	930.20	Joback Method
cpg	1169.95	J/molxK	965.13	Joback Method
cpg	1185.94	J/molxK	1000.06	Joback Method
cpg	1200.62	J/molxK	1034.99	Joback Method
cpg	1214.05	J/molxK	1069.92	Joback Method
cpg	1226.25	J/molxK	1104.85	Joback Method
cpg	1237.26	J/molxK	1139.78	Joback Method
dvisc	0.0004061	Paxs	541.86	Joback Method

dvisc	0.0002054	Paxs	606.58	Joback Method
dvisc	0.0001185	Paxs	671.31	Joback Method
dvisc	0.0000753	Paxs	736.03	Joback Method
dvisc	0.0000515	Paxs	800.75	Joback Method
dvisc	0.0000373	Paxs	865.48	Joback Method
dvisc	0.0000282	Paxs	930.20	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=U349774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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