

Adipic acid, 8-chlorooctyl nonyl ester

Inchi:	InChI=1S/C23H43ClO4/c1-2-3-4-5-7-10-15-20-27-22(25)17-12-13-18-23(26)28-21-16-11
InchiKey:	XEEUDGVMXDHCOZ-UHFFFAOYSA-N
Formula:	C23H43ClO4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	419.04

Physical Properties

Property code	Value	Unit	Source
gf	-336.99	kJ/mol	Joback Method
hf	-1023.39	kJ/mol	Joback Method
hfus	65.10	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.963		Crippen Method
mvol	362.050	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
tb	915.65	K	Joback Method
tc	1122.22	K	Joback Method
tf	523.21	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.72	J/molxK	915.65	Joback Method
cpg	1204.47	J/molxK	950.08	Joback Method
cpg	1221.85	J/molxK	984.51	Joback Method
cpg	1237.89	J/molxK	1018.94	Joback Method
cpg	1252.63	J/molxK	1053.37	Joback Method
cpg	1266.11	J/molxK	1087.80	Joback Method
cpg	1278.36	J/molxK	1122.22	Joback Method
dvisc	0.0004614	Paxs	523.21	Joback Method

dvisc	0.0002249	Paxs	588.62	Joback Method
dvisc	0.0001265	Paxs	654.02	Joback Method
dvisc	0.0000791	Paxs	719.43	Joback Method
dvisc	0.0000534	Paxs	784.84	Joback Method
dvisc	0.0000383	Paxs	850.24	Joback Method
dvisc	0.0000289	Paxs	915.65	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=U349764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvap:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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