

Adipic acid, 8-chlorooctyl octadecyl ester

Inchi:	InChI=1S/C32H61ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-16-19-24-29-36-31(34)26-21
InchiKey:	RZNCOYBKFZZEGV-UHFFFAOYSA-N
Formula:	C32H61ClO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	545.28

Physical Properties

Property code	Value	Unit	Source
gf	-261.21	kJ/mol	Joback Method
hf	-1209.15	kJ/mol	Joback Method
hfus	88.41	kJ/mol	Joback Method
hvap	109.52	kJ/mol	Joback Method
log10ws	-11.10		Crippen Method
logp	10.474		Crippen Method
mcvol	488.860	ml/mol	McGowan Method
pc	557.56	kPa	Joback Method
tb	1121.57	K	Joback Method
tc	1443.67	K	Joback Method
tf	624.64	K	Joback Method
vc	1.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1764.12	J/molxK	1121.57	Joback Method
cpg	1789.17	J/molxK	1175.25	Joback Method
cpg	1810.79	J/molxK	1228.94	Joback Method
cpg	1829.22	J/molxK	1282.62	Joback Method
cpg	1844.70	J/molxK	1336.31	Joback Method
cpg	1857.46	J/molxK	1389.99	Joback Method
cpg	1867.74	J/molxK	1443.67	Joback Method
dvisc	0.0001361	Paxs	624.64	Joback Method
dvisc	0.0000616	Paxs	707.46	Joback Method
dvisc	0.0000329	Paxs	790.28	Joback Method

dvisc	0.0000198	Paxs	873.11	Joback Method
dvisc	0.0000130	Paxs	955.93	Joback Method
dvisc	0.0000091	Paxs	1038.75	Joback Method
dvisc	0.0000068	Paxs	1121.57	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=U349773&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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