

Adipic acid, 10-chlorodecyl tridecyl ester

Inchi:	InChI=1S/C29H55ClO4/c1-2-3-4-5-6-7-8-10-13-16-21-26-33-28(31)23-18-19-24-29(32)30
InchiKey:	KQYRXRDTZFRSKQ-UHFFFAOYSA-N
Formula:	C29H55ClO4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCCCCCI
Mol. weight [g/mol]:	503.20

Physical Properties

Property code	Value	Unit	Source
gf	-286.47	kJ/mol	Joback Method
hf	-1147.23	kJ/mol	Joback Method
hfus	80.64	kJ/mol	Joback Method
hvap	102.84	kJ/mol	Joback Method
log10ws	-9.84		Crippen Method
logp	9.304		Crippen Method
mvol	446.590	ml/mol	McGowan Method
pc	641.90	kPa	Joback Method
rinpol	3558.00		NIST Webbook
tb	1052.93	K	Joback Method
tc	1322.23	K	Joback Method
tf	590.83	K	Joback Method
vc	1.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1568.65	J/molxK	1052.93	Joback Method
cpg	1591.19	J/molxK	1097.81	Joback Method
cpg	1611.29	J/molxK	1142.70	Joback Method
cpg	1629.07	J/molxK	1187.58	Joback Method
cpg	1644.63	J/molxK	1232.46	Joback Method
cpg	1658.10	J/molxK	1277.35	Joback Method
cpg	1669.60	J/molxK	1322.23	Joback Method
dvisc	0.0002084	Paxs	590.83	Joback Method
dvisc	0.0000964	Paxs	667.85	Joback Method

dvisc	0.0000523	Paxs	744.86	Joback Method
dvisc	0.0000318	Paxs	821.88	Joback Method
dvisc	0.0000211	Paxs	898.90	Joback Method
dvisc	0.0000149	Paxs	975.91	Joback Method
dvisc	0.0000111	Paxs	1052.93	Joback Method

Sources

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=U353497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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