

Adipic acid, 10-chlorodecyl octyl ester

Inchi:	InChI=1S/C24H45ClO4/c1-2-3-4-5-11-16-21-28-23(26)18-13-14-19-24(27)29-22-17-12-9
InchiKey:	LIQUVCZJLPZGQN-UHFFFAOYSA-N
Formula:	C24H45ClO4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCCCI
Mol. weight [g/mol]:	433.06

Physical Properties

Property code	Value	Unit	Source
gf	-328.57	kJ/mol	Joback Method
hf	-1044.03	kJ/mol	Joback Method
hfus	67.69	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.353		Crippen Method
mvol	376.140	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	938.53	K	Joback Method
tc	1152.36	K	Joback Method
tf	534.48	K	Joback Method
vc	1.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.50	J/molxK	938.53	Joback Method
cpg	1267.78	J/molxK	974.17	Joback Method
cpg	1285.57	J/molxK	1009.81	Joback Method
cpg	1301.90	J/molxK	1045.44	Joback Method
cpg	1316.83	J/molxK	1081.08	Joback Method
cpg	1330.39	J/molxK	1116.72	Joback Method
cpg	1342.63	J/molxK	1152.36	Joback Method
dvisc	0.0004067	Paxs	534.48	Joback Method

dvisc	0.0001963	Paxs	601.82	Joback Method
dvisc	0.0001097	Paxs	669.16	Joback Method
dvisc	0.0000682	Paxs	736.50	Joback Method
dvisc	0.0000459	Paxs	803.85	Joback Method
dvisc	0.0000329	Paxs	871.19	Joback Method
dvisc	0.0000247	Paxs	938.53	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=U353492&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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