Adipic acid, 2-chloropropyl hexadecyl ester

Inchi: InChI=1S/C25H47ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-29-24(27)19-16-17-20
InchiKey: ITAUICWLDAISFM-UHFFFAOYSA-N
Formula: C25H47ClO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 447.09

Physical Properties

Property code	Value	Unit	Source
gf	-322.59	kJ/mol	Joback Method
hf	-1069.95	kJ/mol	Joback Method
hfus	66.75	kJ/mol	Joback Method
hvap	93.55	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.742		Crippen Method
mcvol	390.230	ml/mol	McGowan Method
pc	791.26	kPa	Joback Method
rinpol	3036.00		NIST Webbook
tb	960.97	K	Joback Method
tc	1181.74	K	Joback Method
tf	530.75	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1312.13	J/mol×K	960.97	Joback Method
cpg	1331.81	J/mol×K	997.77	Joback Method
cpg	1349.86	J/mol×K	1034.56	Joback Method
cpg	1366.33	J/mol×K	1071.36	Joback Method
cpg	1381.28	J/mol×K	1108.15	Joback Method
cpg	1394.75	J/mol×K	1144.95	Joback Method
cpg	1406.80	J/mol×K	1181.74	Joback Method
dvisc	0.0004039	Pa×s	530.75	Joback Method
dvisc	0.0001798	Pa×s	602.45	Joback Method

dvisc	0.0000950	Pa×s	674.16	Joback Method
dvisc	0.0000568	Pa×s	745.86	Joback Method
dvisc	0.0000372	Pa×s	817.56	Joback Method
dvisc	0.0000260	Pa×s	889.27	Joback Method
dvisc	0.0000192	Pa×s	960.97	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=U353552&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