Adipic acid, isohexyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C18H23Cl3O4/c1-12(2)6-5-11-24-15(22)7-3-4-8-16(23)25-18-14(20)10-9-13(19

InchiKey: FZRVKTBSBYZHSS-UHFFFAOYSA-N

Formula: C18H23Cl3O4

SMILES: CC(C)CCCOC(=O)CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl

Mol. weight [g/mol]: 409.73

Physical Properties

Property code	Value	Unit	Source
gf	-321.87	kJ/mol	Joback Method
hf	-754.83	kJ/mol	Joback Method
hfus	49.89	kJ/mol	Joback Method
hvap	91.00	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.092		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2706.00		NIST Webbook
tb	917.29	K	Joback Method
tc	1134.50	K	Joback Method
tf	575.68	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.79	J/mol×K	917.29	Joback Method
cpg	846.87	J/mol×K	953.49	Joback Method
cpg	857.80	J/mol×K	989.69	Joback Method
cpg	867.60	J/mol×K	1025.89	Joback Method
cpg	876.27	J/mol×K	1062.09	Joback Method
cpg	883.83	J/mol×K	1098.30	Joback Method
cpg	890.30	J/mol×K	1134.50	Joback Method
dvisc	0.0003394	Pa×s	575.68	Joback Method
dvisc	0.0002067	Pa×s	632.62	Joback Method

dvisc	0.0001366	Pa×s	689.55	Joback Method
dvisc	0.0000962	Pa×s	746.49	Joback Method
dvisc	0.0000711	Pa×s	803.42	Joback Method
dvisc	0.0000548	Pa×s	860.36	Joback Method
dvisc	0.0000436	Pa×s	917.29	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=U353936&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