Adipic acid, isobutyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H19Cl3O4/c1-10(2)9-22-15(20)5-3-4-6-16(21)23-14-8-12(18)11(17)7-13(14

InchiKey: VTWBJIHSUCCXGM-UHFFFAOYSA-N

Formula: C16H19Cl3O4

SMILES: CC(C)COC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 381.68

Physical Properties

Property code	Value	Unit	Source
gf	-338.71	kJ/mol	Joback Method
hf	-713.55	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	86.55	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.312		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	871.53	K	Joback Method
tc	1089.08	K	Joback Method
tf	553.14	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.95	J/mol×K	871.53	Joback Method
cpg	768.76	J/mol×K	1052.82	Joback Method
cpg	761.28	J/mol×K	1016.56	Joback Method
cpg	752.77	J/mol×K	980.31	Joback Method
cpg	743.22	J/mol×K	944.05	Joback Method
cpg	732.62	J/mol×K	907.79	Joback Method
cpg	775.20	J/mol×K	1089.08	Joback Method
dvisc	0.0000584	Pa×s	871.53	Joback Method

dvisc	0.0000729	Pa×s	818.46	Joback Method
dvisc	0.0000939	Pa×s	765.40	Joback Method
dvisc	0.0001255	Pa×s	712.34	Joback Method
dvisc	0.0001759	Pa×s	659.27	Joback Method
dvisc	0.0002614	Pa×s	606.20	Joback Method
dvisc	0.0004193	Pa×s	553.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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