

Adipic acid, isobutyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C16H19Cl3O4/c1-10(2)9-22-14(20)5-3-4-6-15(21)23-11-7-12(17)16(19)13(18)
InchiKey:	MWJQGLPLLVLPA-UHFFFAOYSA-N
Formula:	C16H19Cl3O4
SMILES:	CC(C)COC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
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
mvol	264.140	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2569.00		NIST Webbook
tb	871.53	K	Joback Method
tc	1089.08	K	Joback Method
tf	553.14	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.95	J/molxK	871.53	Joback Method
cpg	732.62	J/molxK	907.79	Joback Method
cpg	743.22	J/molxK	944.05	Joback Method
cpg	752.77	J/molxK	980.31	Joback Method
cpg	761.28	J/molxK	1016.56	Joback Method
cpg	768.76	J/molxK	1052.82	Joback Method
cpg	775.20	J/molxK	1089.08	Joback Method
dvisc	0.0004193	Paxs	553.14	Joback Method
dvisc	0.0002614	Paxs	606.20	Joback Method

dvisc	0.0001759	Paxs	659.27	Joback Method
dvisc	0.0001255	Paxs	712.34	Joback Method
dvisc	0.0000939	Paxs	765.40	Joback Method
dvisc	0.0000729	Paxs	818.46	Joback Method
dvisc	0.0000584	Paxs	871.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U353906&Units=SI

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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