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

Inchi: InChI=1S/C16H19Cl3O4/c1-2-3-10-22-13(20)6-4-5-7-14(21)23-16-12(18)9-8-11(17)15(16
InchiKey: PTWJDLLAECRXSU-UHFFFAOYSA-N
Formula: C16H19Cl3O4
SMILES: CCCCOC(=O)CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 381.68

Physical Properties

Property code	Value	Unit	Source
gf	-336.27	kJ/mol	Joback Method
hf	-708.27	kJ/mol	Joback Method
hfus	48.23	kJ/mol	Joback Method
hvap	86.94	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.456		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2541.00		NIST Webbook
tb	871.97	K	Joback Method
tc	1087.15	K	Joback Method
tf	568.14	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.38	J/mol×K	871.97	Joback Method
cpg	731.95	J/mol×K	907.83	Joback Method
cpg	742.49	J/mol×K	943.70	Joback Method
cpg	752.01	J/mol×K	979.56	Joback Method
cpg	760.53	J/mol×K	1015.42	Joback Method
cpg	768.04	J/mol×K	1051.29	Joback Method
cpg	774.56	J/mol×K	1087.15	Joback Method
dvisc	0.0003890	Pa×s	568.14	Joback Method
dvisc	0.0002544	Pa×s	618.78	Joback Method

dvisc	0.0001774	Pa×s	669.42	Joback Method
dvisc	0.0001302	Pa×s	720.05	Joback Method
dvisc	0.0000995	Pa×s	770.69	Joback Method
dvisc	0.0000786	Pa×s	821.33	Joback Method
dvisc	0.0000638	Pa×s	871.97	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=U353934&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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