

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

Inchi:	InChI=1S/C16H19Cl3O4/c1-2-3-8-22-14(20)6-4-5-7-15(21)23-11-9-12(17)16(19)13(18)10
InchiKey:	IPEQKDRIXFUVBZ-UHFFFAOYSA-N
Formula:	C16H19Cl3O4
SMILES:	CCCCOC(=O)CCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
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
mvol	264.140	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	871.97	K	Joback Method
tc	1087.15	K	Joback Method
tf	568.14	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.38	J/molxK	871.97	Joback Method
cpg	731.95	J/molxK	907.83	Joback Method
cpg	742.49	J/molxK	943.70	Joback Method
cpg	752.01	J/molxK	979.56	Joback Method
cpg	760.53	J/molxK	1015.42	Joback Method
cpg	768.04	J/molxK	1051.29	Joback Method
cpg	774.56	J/molxK	1087.15	Joback Method
dvisc	0.0003890	Paxs	568.14	Joback Method

dvisc	0.0002544	Paxs	618.78	Joback Method
dvisc	0.0001774	Paxs	669.42	Joback Method
dvisc	0.0001302	Paxs	720.05	Joback Method
dvisc	0.0000995	Paxs	770.69	Joback Method
dvisc	0.0000786	Paxs	821.33	Joback Method
dvisc	0.0000638	Paxs	871.97	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=U353907&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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