

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

Inchi:	InChI=1S/C17H21Cl3O4/c1-2-3-6-11-23-14(21)7-4-5-8-15(22)24-17-13(19)10-9-12(18)16
InchiKey:	PCGPJCUVSRSNJK-UHFFFAOYSA-N
Formula:	C17H21Cl3O4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	395.70

Physical Properties

Property code	Value	Unit	Source
gf	-327.85	kJ/mol	Joback Method
hf	-728.91	kJ/mol	Joback Method
hfus	50.82	kJ/mol	Joback Method
hvap	89.16	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.846		Crippen Method
mcvol	278.230	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinqol	2644.00		NIST Webbook
tb	894.85	K	Joback Method
tc	1109.82	K	Joback Method
tf	579.41	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.95	J/molxK	894.85	Joback Method
cpg	788.76	J/molxK	930.68	Joback Method
cpg	799.50	J/molxK	966.51	Joback Method
cpg	809.18	J/molxK	1002.34	Joback Method
cpg	817.80	J/molxK	1038.17	Joback Method
cpg	825.39	J/molxK	1073.99	Joback Method
cpg	831.96	J/molxK	1109.82	Joback Method
dvisc	0.0003515	Paxs	579.41	Joback Method
dvisc	0.0002271	Paxs	631.98	Joback Method

dvisc	0.0001570	Paxs	684.56	Joback Method
dvisc	0.0001143	Paxs	737.13	Joback Method
dvisc	0.0000869	Paxs	789.70	Joback Method
dvisc	0.0000683	Paxs	842.28	Joback Method
dvisc	0.0000553	Paxs	894.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353935&Units=SI
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

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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