

Adipic acid, butyl 2,3,4,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C16H18Cl4O4/c1-2-3-8-23-12(21)6-4-5-7-13(22)24-16-11(18)9-10(17)14(19)15
InchiKey:	MTGQBSMKIFMBDI-UHFFFAOYSA-N
Formula:	C16H18Cl4O4
SMILES:	CCCCOC(=O)CCCCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	416.12

Physical Properties

Property code	Value	Unit	Source
gf	-357.83	kJ/mol	Joback Method
hf	-735.48	kJ/mol	Joback Method
hfus	52.04	kJ/mol	Joback Method
hvap	91.99	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.109		Crippen Method
mcvol	276.380	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinsol	2703.00		NIST Webbook
tb	914.38	K	Joback Method
tc	1134.72	K	Joback Method
tf	610.58	K	Joback Method
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.79	J/molxK	914.38	Joback Method
cpg	780.84	J/molxK	1097.99	Joback Method
cpg	774.74	J/molxK	1061.27	Joback Method
cpg	767.59	J/molxK	1024.55	Joback Method
cpg	759.38	J/molxK	987.83	Joback Method
cpg	750.12	J/molxK	951.10	Joback Method
cpg	785.90	J/molxK	1134.72	Joback Method
dvisc	0.0000555	Paxs	914.38	Joback Method
dvisc	0.0000676	Paxs	863.75	Joback Method

dvisc	0.0000843	Paxs	813.11	Joback Method
dvisc	0.0001083	Paxs	762.48	Joback Method
dvisc	0.0001442	Paxs	711.85	Joback Method
dvisc	0.0002006	Paxs	661.21	Joback Method
dvisc	0.0002947	Paxs	610.58	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=U353914&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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