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

Inchi: InChI=1S/C18H22Cl4O4/c1-2-3-4-7-10-25-14(23)8-5-6-9-15(24)26-18-13(20)11-12(19)16

InchiKey: LSFZFXCVXXXJSC-UHFFFAOYSA-N

Formula: C18H22Cl4O4

SMILES: CCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 444.18

Physical Properties

Property code	Value	Unit	Source
gf	-340.99	kJ/mol	Joback Method
hf	-776.76	kJ/mol	Joback Method
hfus	57.22	kJ/mol	Joback Method
hvap	96.44	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.889		Crippen Method
mcvol	304.560	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook
tb	960.14	K	Joback Method
tc	1181.98	K	Joback Method
tf	633.12	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.87	J/mol×K	960.14	Joback Method
cpg	864.61	J/mol×K	997.11	Joback Method
cpg	874.18	J/mol×K	1034.09	Joback Method
cpg	882.58	J/mol×K	1071.06	Joback Method
cpg	889.83	J/mol×K	1108.03	Joback Method
cpg	895.95	J/mol×K	1145.00	Joback Method
cpg	900.93	J/mol×K	1181.98	Joback Method
dvisc	0.0002379	Pa×s	633.12	Joback Method

dvisc	0.0001583	Pa×s	687.62	Joback Method
dvisc	0.0001118	Pa×s	742.13	Joback Method
dvisc	0.0000828	Pa×s	796.63	Joback Method
dvisc	0.0000637	Pa×s	851.13	Joback Method
dvisc	0.0000506	Pa×s	905.64	Joback Method
dvisc	0.0000413	Pa×s	960.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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