

Adipic acid, propyl 2,3,5,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C15H16Cl4O4/c1-2-7-22-11(20)5-3-4-6-12(21)23-15-13(18)9(16)8-10(17)14(19)
InchiKey:	HYQUZSJHYOVKFW-UHFFFAOYSA-N
Formula:	C15H16Cl4O4
SMILES:	CCCOC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	402.10

Physical Properties

Property code	Value	Unit	Source
gf	-366.25	kJ/mol	Joback Method
hf	-714.84	kJ/mol	Joback Method
hfus	49.45	kJ/mol	Joback Method
hvap	89.76	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.719		Crippen Method
mvol	262.290	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	891.50	K	Joback Method
tc	1112.28	K	Joback Method
tf	599.31	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.84	J/molxK	891.50	Joback Method
cpg	724.08	J/molxK	1075.49	Joback Method
cpg	718.05	J/molxK	1038.69	Joback Method
cpg	711.02	J/molxK	1001.89	Joback Method
cpg	702.97	J/molxK	965.09	Joback Method
cpg	693.91	J/molxK	928.30	Joback Method
cpg	729.10	J/molxK	1112.28	Joback Method
dvisc	0.0000642	Paxs	891.50	Joback Method

dvisc	0.0000779	Paxs	842.80	Joback Method
dvisc	0.0000967	Paxs	794.10	Joback Method
dvisc	0.0001234	Paxs	745.40	Joback Method
dvisc	0.0001631	Paxs	696.71	Joback Method
dvisc	0.0002248	Paxs	648.01	Joback Method
dvisc	0.0003264	Paxs	599.31	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=U353946&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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