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

Inchi: InChI=1S/C20H26Cl4O4/c1-2-3-4-5-6-9-12-27-16(25)10-7-8-11-17(26)28-20-15(22)13-14

InchiKey: LFMGPCYJMDMKDU-UHFFFAOYSA-N

Formula: C20H26Cl4O4

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

Mol. weight [g/mol]: 472.23

Physical Properties

Property code	Value	Unit	Source
gf	-324.15	kJ/mol	Joback Method
hf	-818.04	kJ/mol	Joback Method
hfus	62.40	kJ/mol	Joback Method
hvap	100.89	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.670		Crippen Method
mcvol	332.740	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	3118.00		NIST Webbook
rinpol	3118.00		NIST Webbook
tb	1005.90	K	Joback Method
tc	1232.79	K	Joback Method
tf	655.66	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.43	J/mol×K	1005.90	Joback Method
cpg	1012.90	J/mol×K	1194.98	Joback Method
cpg	1006.95	J/mol×K	1157.16	Joback Method
cpg	999.74	J/mol×K	1119.35	Joback Method
cpg	991.27	J/mol×K	1081.53	Joback Method
cpg	981.50	J/mol×K	1043.72	Joback Method
cpg	1017.62	J/mol×K	1232.79	Joback Method
dvisc	0.0000305	Pa×s	1005.90	Joback Method

dvisc	0.0000376	Pa×s	947.53	Joback Method
dvisc	0.0000478	Pa×s	889.15	Joback Method
dvisc	0.0000627	Pa×s	830.78	Joback Method
dvisc	0.0000858	Pa×s	772.41	Joback Method
dvisc	0.0001235	Pa×s	714.03	Joback Method
dvisc	0.0001897	Pa×s	655.66	Joback Method

Sources

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=U353919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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