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

Inchi: InChI=1S/C19H24Cl4O4/c1-2-3-4-5-8-11-26-15(24)9-6-7-10-16(25)27-19-14(21)12-13(20

InchiKey: YMRJIUQPUXXBDV-UHFFFAOYSA-N

Formula: C19H24Cl4O4

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

Mol. weight [g/mol]: 458.20

Physical Properties

Property code	Value	Unit	Source
gf	-332.57	kJ/mol	Joback Method
hf	-797.40	kJ/mol	Joback Method
hfus	59.81	kJ/mol	Joback Method
hvap	98.66	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.280		Crippen Method
mcvol	318.650	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	983.02	K	Joback Method
tc	1206.91	K	Joback Method
tf	644.39	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.87	J/mol×K	983.02	Joback Method
cpg	922.78	J/mol×K	1020.34	Joback Method
cpg	932.46	J/mol×K	1057.65	Joback Method
cpg	940.91	J/mol×K	1094.97	Joback Method
cpg	948.16	J/mol×K	1132.28	Joback Method
cpg	954.21	J/mol×K	1169.60	Joback Method
cpg	959.09	J/mol×K	1206.91	Joback Method
dvisc	0.0002127	Pa×s	644.39	Joback Method

dvisc	0.0001400	Pa×s	700.83	Joback Method
dvisc	0.0000980	Pa×s	757.27	Joback Method
dvisc	0.0000721	Pa×s	813.71	Joback Method
dvisc	0.0000552	Pa×s	870.14	Joback Method
dvisc	0.0000437	Pa×s	926.58	Joback Method
dvisc	0.0000355	Pa×s	983.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353918&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

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