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

Inchi: InChI=1S/C16H18Cl4O4/c1-2-3-4-5-8-23-12(21)6-7-13(22)24-16-11(18)9-10(17)14(19)15

InchiKey: UWAQLHSZIULLMW-UHFFFAOYSA-N

Formula: C16H18Cl4O4

SMILES: CCCCCCOC(=O)CCC(=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
rinpol	2667.00		NIST Webbook
tb	914.38	K	Joback Method
tc	1134.72	K	Joback Method
tf	610.58	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.79	J/mol×K	914.38	Joback Method
cpg	750.12	J/mol×K	951.10	Joback Method
cpg	759.38	J/mol×K	987.83	Joback Method
cpg	767.59	J/mol×K	1024.55	Joback Method
cpg	774.74	J/mol×K	1061.27	Joback Method
cpg	780.84	J/mol×K	1097.99	Joback Method
cpg	785.90	J/mol×K	1134.72	Joback Method
dvisc	0.0002947	Pa×s	610.58	Joback Method
dvisc	0.0002006	Pa×s	661.21	Joback Method

dvisc	0.0001442	Pa×s	711.85	Joback Method
dvisc	0.0001083	Pa×s	762.48	Joback Method
dvisc	0.0000843	Pa×s	813.11	Joback Method
dvisc	0.0000676	Pa×s	863.75	Joback Method
dvisc	0.0000555	Pa×s	914.38	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U349678&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