Succinic acid, 2-methylpent-3-yl pentachlorophenyl ester

Inchi: InChI=1S/C16H17Cl5O4/c1-4-8(7(2)3)24-9(22)5-6-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: YSEMQQRTRMGPRF-UHFFFAOYSA-N

Formula: C16H17Cl5O4

SMILES: CCC(OC(=O)CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)C(C)C

Mol. weight [g/mol]: 450.57

Physical Properties

Property code	Value	Unit	Source
gf	-384.27	kJ/mol	Joback Method
hf	-773.25	kJ/mol	Joback Method
hfus	48.80	kJ/mol	Joback Method
hvap	96.26	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.617		Crippen Method
mcvol	288.620	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	955.91	K	Joback Method
tc	1185.64	K	Joback Method
tf	623.02	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.16	J/mol×K	955.91	Joback Method
cpg	767.25	J/mol×K	994.20	Joback Method
cpg	775.16	J/mol×K	1032.49	Joback Method
cpg	781.88	J/mol×K	1070.78	Joback Method
cpg	787.43	J/mol×K	1109.06	Joback Method
cpg	791.79	J/mol×K	1147.35	Joback Method
cpg	794.97	J/mol×K	1185.64	Joback Method
dvisc	0.0002475	Pa×s	623.02	Joback Method

dvisc	0.0001613	Pa×s	678.50	Joback Method
dvisc	0.0001121	Pa×s	733.98	Joback Method
dvisc	0.0000820	Pa×s	789.47	Joback Method
dvisc	0.0000625	Pa×s	844.95	Joback Method
dvisc	0.0000493	Pa×s	900.43	Joback Method
dvisc	0.0000399	Pa×s	955.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390047&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