Succinic acid, hept-2-yl pentachlorophenyl ester

Inchi: InChI=1S/C17H19Cl5O4/c1-3-4-5-6-9(2)25-10(23)7-8-11(24)26-17-15(21)13(19)12(18)14

InchiKey: HPKKANURHIOVMQ-UHFFFAOYSA-N

Formula: C17H19Cl5O4

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

Mol. weight [g/mol]: 464.60

Physical Properties

Property code	Value	Unit	Source
gf	-373.41	kJ/mol	Joback Method
hf	-788.61	kJ/mol	Joback Method
hfus	54.92	kJ/mol	Joback Method
hvap	98.87	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.151		Crippen Method
mcvol	302.710	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	979.23	K	Joback Method
tc	1207.53	K	Joback Method
tf	649.29	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.39	J/mol×K	979.23	Joback Method
cpg	823.62	J/mol×K	1017.28	Joback Method
cpg	831.64	J/mol×K	1055.33	Joback Method
cpg	838.47	J/mol×K	1093.38	Joback Method
cpg	844.10	J/mol×K	1131.43	Joback Method
cpg	848.53	J/mol×K	1169.48	Joback Method
cpg	851.77	J/mol×K	1207.53	Joback Method
dvisc	0.0002110	Pa×s	649.29	Joback Method

dvisc	0.0001416	Pa×s	704.28	Joback Method
dvisc	0.0001006	Pa×s	759.27	Joback Method
dvisc	0.0000749	Pa×s	814.26	Joback Method
dvisc	0.0000579	Pa×s	869.25	Joback Method
dvisc	0.0000461	Pa×s	924.24	Joback Method
dvisc	0.0000377	Pa×s	979.23	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=U390049&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