Succinic acid, cyclohexylmethyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H19Cl3O4/c18-12-8-13(19)17(14(20)9-12)24-16(22)7-6-15(21)23-10-11-4-

InchiKey: DNDGCGKUPLINLK-UHFFFAOYSA-N

Formula: C17H19Cl3O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC1CCCCC1

Mol. weight [g/mol]: 393.69

Physical Properties

Property code	Value	Unit	Source
gf	-303.40	kJ/mol	Joback Method
hf	-674.59	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	89.59	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.456		Crippen Method
mcvol	267.370	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	914.40	K	Joback Method
tc	1150.72	K	Joback Method
tf	586.79	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.17	J/mol×K	914.40	Joback Method
cpg	781.28	J/mol×K	953.79	Joback Method
cpg	791.95	J/mol×K	993.17	Joback Method
cpg	801.18	J/mol×K	1032.56	Joback Method
cpg	809.00	J/mol×K	1071.94	Joback Method
cpg	815.41	J/mol×K	1111.33	Joback Method
cpg	820.45	J/mol×K	1150.72	Joback Method
dvisc	0.0003946	Pa×s	586.79	Joback Method

dvisc	0.0002493	Pa×s	641.39	Joback Method
dvisc	0.0001693	Pa×s	695.99	Joback Method
dvisc	0.0001216	Pa×s	750.60	Joback Method
dvisc	0.0000913	Pa×s	805.20	Joback Method
dvisc	0.0000712	Pa×s	859.80	Joback Method
dvisc	0.0000571	Pa×s	914.40	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=U390278&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