Succinic acid, 2,2-dichloroethyl 4-bromophenyl ester

Inchi: InChI=1S/C12H11BrCl2O4/c13-8-1-3-9(4-2-8)19-12(17)6-5-11(16)18-7-10(14)15/h1-4,10

InchiKey: ARBSHKNAUOLACR-UHFFFAOYSA-N

Formula: C12H11BrCl2O4

SMILES: O=C(CCC(=O)Oc1ccc(Br)cc1)OCC(Cl)Cl

Mol. weight [g/mol]: 370.02

Physical Properties

Property code	Value	Unit	Source
gf	-326.88	kJ/mol	Joback Method
hf	-565.98	kJ/mol	Joback Method
hfus	36.22	kJ/mol	Joback Method
hvap	78.37	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.482		Crippen Method
mcvol	213.040	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	2361.00		NIST Webbook
tb	798.78	K	Joback Method
tc	1030.49	K	Joback Method
tf	512.90	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.88	J/mol×K	798.78	Joback Method
cpg	525.87	J/mol×K	837.40	Joback Method
cpg	534.93	J/mol×K	876.02	Joback Method
cpg	543.09	J/mol×K	914.63	Joback Method
cpg	550.38	J/mol×K	953.25	Joback Method
cpg	556.80	J/mol×K	991.87	Joback Method
cpg	562.38	J/mol×K	1030.49	Joback Method
dvisc	0.0006662	Pa×s	512.90	Joback Method
dvisc	0.0004172	Pa×s	560.55	Joback Method

dvisc	0.0002811	Pa×s	608.19	Joback Method
dvisc	0.0002006	Pa×s	655.84	Joback Method
dvisc	0.0001499	Pa×s	703.49	Joback Method
dvisc	0.0001162	Pa×s	751.13	Joback Method
dvisc	0.0000928	Pa×s	798.78	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=U389822&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