Succinic acid, di(4-chloro-2-methylbenzyl) ester

Inchi: InChI=1S/C20H20Cl2O4/c1-13-9-17(21)5-3-15(13)11-25-19(23)7-8-20(24)26-12-16-4-6-1

InchiKey: QBHDOEVLWLVTRN-UHFFFAOYSA-N

Formula: C20H20Cl2O4

SMILES: Cc1cc(Cl)ccc1COC(=O)CCC(=O)OCc1ccc(Cl)cc1C

Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	-187.88	kJ/mol	Joback Method
hf	-550.03	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	94.40	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.177		Crippen Method
mcvol	284.500	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2952.00		NIST Webbook
rinpol	2952.00		NIST Webbook
tb	957.72	K	Joback Method
tc	1191.17	K	Joback Method
tf	622.24	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.52	J/mol×K	957.72	Joback Method
cpg	832.62	J/mol×K	996.63	Joback Method
cpg	842.39	J/mol×K	1035.54	Joback Method
cpg	850.87	J/mol×K	1074.45	Joback Method
cpg	858.09	J/mol×K	1113.35	Joback Method
cpg	864.06	J/mol×K	1152.26	Joback Method
cpg	868.80	J/mol×K	1191.17	Joback Method
dvisc	0.0002590	Pa×s	622.24	Joback Method

dvisc	0.0001710	Pa×s	678.15	Joback Method
dvisc	0.0001202	Pa×s	734.07	Joback Method
dvisc	0.0000889	Pa×s	789.98	Joback Method
dvisc	0.0000684	Pa×s	845.89	Joback Method
dvisc	0.0000543	Pa×s	901.81	Joback Method
dvisc	0.0000444	Pa×s	957.72	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=U380882&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

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