Succinic acid, di(2-methoxy-4-chlorobenzyl) ester

Inchi: InChI=1S/C20H20Cl2O6/c1-25-17-9-15(21)5-3-13(17)11-27-19(23)7-8-20(24)28-12-14-4

InchiKey: TYGYKEIGXQMKCZ-UHFFFAOYSA-N

Formula: C20H20Cl2O6

SMILES: COc1cc(Cl)ccc1COC(=O)CCC(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 427.27

Physical Properties

Property code	Value	Unit	Source
gf	-397.88	kJ/mol	Joback Method
hf	-814.47	kJ/mol	Joback Method
hfus	50.43	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.577		Crippen Method
mcvol	296.240	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	3103.00		NIST Webbook
rinpol	3103.00		NIST Webbook
tb	1002.56	K	Joback Method
tc	1236.99	K	Joback Method
tf	666.70	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.16	J/mol×K	1002.56	Joback Method
cpg	899.26	J/mol×K	1197.92	Joback Method
cpg	897.03	J/mol×K	1158.84	Joback Method
cpg	893.09	J/mol×K	1119.77	Joback Method
cpg	887.46	J/mol×K	1080.70	Joback Method
cpg	880.14	J/mol×K	1041.63	Joback Method
cpg	899.75	J/mol×K	1236.99	Joback Method
dvisc	0.0000244	Pa×s	1002.56	Joback Method

dvisc	0.0000298	Pa×s	946.58	Joback Method
dvisc	0.0000373	Pa×s	890.61	Joback Method
dvisc	0.0000481	Pa×s	834.63	Joback Method
dvisc	0.0000643	Pa×s	778.65	Joback Method
dvisc	0.0000901	Pa×s	722.68	Joback Method
dvisc	0.0001333	Pa×s	666.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380856&Units=SI
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

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