

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.16	J/molxK	1002.56	Joback Method
cpg	880.14	J/molxK	1041.63	Joback Method
cpg	887.46	J/molxK	1080.70	Joback Method
cpg	893.09	J/molxK	1119.77	Joback Method
cpg	897.03	J/molxK	1158.84	Joback Method
cpg	899.26	J/molxK	1197.92	Joback Method
cpg	899.75	J/molxK	1236.99	Joback Method
dvisc	0.0001333	Paxs	666.70	Joback Method

dvisc	0.0000901	Paxs	722.68	Joback Method
dvisc	0.0000643	Paxs	778.65	Joback Method
dvisc	0.0000481	Paxs	834.63	Joback Method
dvisc	0.0000373	Paxs	890.61	Joback Method
dvisc	0.0000298	Paxs	946.58	Joback Method
dvisc	0.0000244	Paxs	1002.56	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/ci9903071
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

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