

Succinic acid, 2-methoxy-4-chlorobenzyl octyl ester

Inchi:	InChI=1S/C20H29ClO5/c1-3-4-5-6-7-8-13-25-19(22)11-12-20(23)26-15-16-9-10-17(21)14
InchiKey:	HHQYDWQQCZODGS-UHFFFAOYSA-N
Formula:	C20H29ClO5
SMILES:	CCCCCCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	384.89

Physical Properties

Property code	Value	Unit	Source
gf	-374.10	kJ/mol	Joback Method
hf	-880.10	kJ/mol	Joback Method
hfus	51.78	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.076		Crippen Method
mvol	301.890	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2737.00		NIST Webbook
rinpol	2737.00		NIST Webbook
tb	906.07	K	Joback Method
tc	1114.34	K	Joback Method
tf	563.09	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.56	J/molxK	906.07	Joback Method
cpg	991.44	J/molxK	1079.63	Joback Method
cpg	982.19	J/molxK	1044.92	Joback Method
cpg	971.68	J/molxK	1010.21	Joback Method
cpg	959.91	J/molxK	975.49	Joback Method
cpg	946.87	J/molxK	940.78	Joback Method
cpg	999.45	J/molxK	1114.34	Joback Method
dvisc	0.0000358	Paxs	906.07	Joback Method

dvisc	0.0000453	Paxs	848.91	Joback Method
dvisc	0.0000592	Paxs	791.74	Joback Method
dvisc	0.0000807	Paxs	734.58	Joback Method
dvisc	0.0001160	Paxs	677.42	Joback Method
dvisc	0.0001781	Paxs	620.25	Joback Method
dvisc	0.0002985	Paxs	563.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380852&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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