

Succinic acid, di(3-chlorobenzyl) ester

Inchi: InChI=1S/C18H16Cl2O4/c19-15-5-1-3-13(9-15)11-23-17(21)7-8-18(22)24-12-14-4-2-6-10
InchiKey: GUSHJPAYWBYVQE-UHFFFAOYSA-N
Formula: C18H16Cl2O4
SMILES: O=C(CCC(=O)OCc1cccc(Cl)c1)OCc1cccc(Cl)c1
Mol. weight [g/mol]: 367.22

Physical Properties

Property code	Value	Unit	Source
gf	-185.46	kJ/mol	Joback Method
hf	-485.81	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	88.62	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.560		Crippen Method
mvol	256.320	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	902.00	K	Joback Method
tc	1137.10	K	Joback Method
tf	574.66	K	Joback Method
vc	0.974	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.95	J/molxK	902.00	Joback Method
cpg	722.05	J/molxK	941.18	Joback Method
cpg	731.92	J/molxK	980.37	Joback Method
cpg	740.60	J/molxK	1019.55	Joback Method
cpg	748.13	J/molxK	1058.74	Joback Method
cpg	754.54	J/molxK	1097.92	Joback Method
cpg	759.86	J/molxK	1137.10	Joback Method
dvisc	0.0003880	Paxs	574.66	Joback Method

dvisc	0.0002449	Paxs	629.22	Joback Method
dvisc	0.0001664	Paxs	683.77	Joback Method
dvisc	0.0001197	Paxs	738.33	Joback Method
dvisc	0.0000901	Paxs	792.89	Joback Method
dvisc	0.0000703	Paxs	847.44	Joback Method
dvisc	0.0000566	Paxs	902.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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