

Succinic acid, di(2,4-dichlorobenzyl) ester

Inchi:	InChI=1S/C18H14Cl4O4/c19-13-3-1-11(15(21)7-13)9-25-17(23)5-6-18(24)26-10-12-2-4-
InchiKey:	VBOPUIURWHMRKV-UHFFFAOYSA-N
Formula:	C18H14Cl4O4
SMILES:	O=C(CCC(=O)OCc1ccc(Cl)cc1Cl)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	436.11

Physical Properties

Property code	Value	Unit	Source
gf	-228.58	kJ/mol	Joback Method
hf	-540.23	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	98.71	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.867		Crippen Method
mvol	280.800	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	3097.00		NIST Webbook
rinpol	3097.00		NIST Webbook
tb	986.82	K	Joback Method
tc	1229.94	K	Joback Method
tf	659.54	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.08	J/molxK	986.82	Joback Method
cpg	772.80	J/molxK	1189.42	Joback Method
cpg	769.44	J/molxK	1148.90	Joback Method
cpg	764.91	J/molxK	1108.38	Joback Method
cpg	759.19	J/molxK	1067.86	Joback Method
cpg	752.26	J/molxK	1027.34	Joback Method
cpg	775.01	J/molxK	1229.94	Joback Method
dvisc	0.0000430	Paxs	986.82	Joback Method

dvisc	0.0000522	Paxs	932.27	Joback Method
dvisc	0.0000650	Paxs	877.73	Joback Method
dvisc	0.0000833	Paxs	823.18	Joback Method
dvisc	0.0001107	Paxs	768.63	Joback Method
dvisc	0.0001534	Paxs	714.09	Joback Method
dvisc	0.0002246	Paxs	659.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381150&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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