

Succinic acid, 3-chlorobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H25ClO4/c1-4-6-16(13(2)3)23-18(21)10-9-17(20)22-12-14-7-5-8-15(19)11-
InchiKey:	JMWMEFALGGZNDH-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	CCCC(OC(=O)CCC(=O)OCc1cccc(Cl)c1)C(C)C
Mol. weight [g/mol]:	340.84

Physical Properties

Property code	Value	Unit	Source
gf	-281.19	kJ/mol	Joback Method
hf	-705.69	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.531		Crippen Method
mvol	267.840	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2287.00		NIST Webbook
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tb	832.03	K	Joback Method
tc	1040.64	K	Joback Method
tf	475.80	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.48	J/molxK	832.03	Joback Method
cpg	804.30	J/molxK	866.80	Joback Method
cpg	817.99	J/molxK	901.57	Joback Method
cpg	830.57	J/molxK	936.33	Joback Method
cpg	842.05	J/molxK	971.10	Joback Method
cpg	852.47	J/molxK	1005.87	Joback Method
cpg	861.84	J/molxK	1040.64	Joback Method
dvisc	0.0007660	Paxs	475.80	Joback Method

dvisc	0.0003832	Paxs	535.17	Joback Method
dvisc	0.0002201	Paxs	594.54	Joback Method
dvisc	0.0001398	Paxs	653.91	Joback Method
dvisc	0.0000958	Paxs	713.29	Joback Method
dvisc	0.0000696	Paxs	772.66	Joback Method
dvisc	0.0000529	Paxs	832.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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