

Succinic acid, cyclohexylmethyl 4-chlorobenzyl ester

Inchi:	InChI=1S/C18H23ClO4/c19-16-8-6-15(7-9-16)13-23-18(21)11-10-17(20)22-12-14-4-2-1-3
InchiKey:	ZEYNDNJCMLEROC-UHFFFAOYSA-N
Formula:	C18H23ClO4
SMILES:	O=C(CCC(=O)OCC1CCCCC1)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	338.83

Physical Properties

Property code	Value	Unit	Source
gf	-251.86	kJ/mol	Joback Method
hf	-640.81	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.287		Crippen Method
mvol	256.980	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	852.46	K	Joback Method
tc	1078.83	K	Joback Method
tf	513.18	K	Joback Method
vc	0.966	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.42	J/molxK	852.46	Joback Method
cpg	797.89	J/molxK	890.19	Joback Method
cpg	811.91	J/molxK	927.92	Joback Method
cpg	824.52	J/molxK	965.64	Joback Method
cpg	835.73	J/molxK	1003.37	Joback Method
cpg	845.59	J/molxK	1041.10	Joback Method
cpg	854.12	J/molxK	1078.83	Joback Method
dvisc	0.0006773	Paxs	513.18	Joback Method

dvisc	0.0003777	Paxs	569.73	Joback Method
dvisc	0.0002341	Paxs	626.27	Joback Method
dvisc	0.0001570	Paxs	682.82	Joback Method
dvisc	0.0001120	Paxs	739.37	Joback Method
dvisc	0.0000838	Paxs	795.91	Joback Method
dvisc	0.0000651	Paxs	852.46	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389677&Units=SI

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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