

Succinic acid, 3-methylbut-2-yl 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-10(2)12(4)20-15(18)7-8-16(19)21-14-6-5-13(17)9-11(14)3/h5-
InchiKey:	KIOLQYBELWVEPW-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	<chem>Cc1cc(Cl)ccc1OC(=O)CCC(=O)OC(C)C(C)C</chem>
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-307.66	kJ/mol	Joback Method
hf	-675.88	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.922		Crippen Method
mvol	239.660	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	791.25	K	Joback Method
tc	1003.34	K	Joback Method
tf	465.78	K	Joback Method
vc	0.908	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.30	J/molxK	791.25	Joback Method
cpg	736.28	J/molxK	967.99	Joback Method
cpg	726.17	J/molxK	932.64	Joback Method
cpg	715.02	J/molxK	897.30	Joback Method
cpg	702.84	J/molxK	861.95	Joback Method
cpg	689.60	J/molxK	826.60	Joback Method
cpg	745.38	J/molxK	1003.34	Joback Method
dvisc	0.0000705	Paxs	791.25	Joback Method

dvisc	0.0000908	Paxs	737.00	Joback Method
dvisc	0.0001219	Paxs	682.76	Joback Method
dvisc	0.0001722	Paxs	628.51	Joback Method
dvisc	0.0002597	Paxs	574.27	Joback Method
dvisc	0.0004265	Paxs	520.02	Joback Method
dvisc	0.0007862	Paxs	465.78	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=U390289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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