

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

Inchi: InChI=1S/C16H21ClO5/c1-10(2)11(3)21-15(18)7-8-16(19)22-13-6-5-12(17)9-14(13)20-4/
InchiKey: NOGMJYGQKLWFNA-UHFFFAOYSA-N
Formula: C16H21ClO5
SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 328.79

Physical Properties

Property code	Value	Unit	Source
gf	-412.66	kJ/mol	Joback Method
hf	-808.10	kJ/mol	Joback Method
hfus	34.37	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.622		Crippen Method
mcvol	245.530	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2249.00		NIST Webbook
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tb	813.67	K	Joback Method
tc	1024.81	K	Joback Method
tf	488.01	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.54	J/molxK	813.67	Joback Method
cpg	716.37	J/molxK	848.86	Joback Method
cpg	729.09	J/molxK	884.05	Joback Method
cpg	740.70	J/molxK	919.24	Joback Method
cpg	751.17	J/molxK	954.43	Joback Method
cpg	760.52	J/molxK	989.62	Joback Method
cpg	768.73	J/molxK	1024.81	Joback Method
dvisc	0.0005523	Paxs	488.01	Joback Method

dvisc	0.0003076	Paxs	542.29	Joback Method
dvisc	0.0001906	Paxs	596.56	Joback Method
dvisc	0.0001279	Paxs	650.84	Joback Method
dvisc	0.0000913	Paxs	705.12	Joback Method
dvisc	0.0000683	Paxs	759.39	Joback Method
dvisc	0.0000532	Paxs	813.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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