Succinic acid, 4-chloro-2-methylbenzyl isobutyl ester

Inchi: InChI=1S/C16H21ClO4/c1-11(2)9-20-15(18)6-7-16(19)21-10-13-4-5-14(17)8-12(13)3/h4-

InchiKey: HBOAPSJXKWSMJI-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: Cc1cc(Cl)ccc1COC(=O)CCC(=O)OCC(C)C

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-305.22	kJ/mol	Joback Method
hf	-670.60	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.671		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	791.69	K	Joback Method
tc	1000.85	K	Joback Method
tf	480.78	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.74	J/mol×K	791.69	Joback Method
cpg	688.84	J/mol×K	826.55	Joback Method
cpg	701.92	J/mol×K	861.41	Joback Method
cpg	713.99	J/mol×K	896.27	Joback Method
cpg	725.06	J/mol×K	931.13	Joback Method
cpg	735.14	J/mol×K	965.99	Joback Method
cpg	744.24	J/mol×K	1000.85	Joback Method
dvisc	0.0006920	Pa×s	480.78	Joback Method

dvisc	0.0004012	Pa×s	532.60	Joback Method
dvisc	0.0002562	Pa×s	584.42	Joback Method
dvisc	0.0001760	Pa×s	636.24	Joback Method
dvisc	0.0001280	Pa×s	688.05	Joback Method
dvisc	0.0000973	Pa×s	739.87	Joback Method
dvisc	0.0000767	Pa×s	791.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380879&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