Succinic acid, isobutyl 2-methoxy-4-chlorobenzyl ester

Inchi: InChI=1S/C16H21ClO5/c1-11(2)9-21-15(18)6-7-16(19)22-10-12-4-5-13(17)8-14(12)20-3/

InchiKey: ORDZBKVLKRGDNJ-UHFFFAOYSA-N

Formula: C16H21ClO5

SMILES: COc1cc(Cl)ccc1COC(=O)CCC(=O)OCC(C)C

Mol. weight [g/mol]: 328.79

Physical Properties

Property code	Value	Unit	Source
gf	-410.22	kJ/mol	Joback Method
hf	-802.82	kJ/mol	Joback Method
hfus	37.89	kJ/mol	Joback Method
hvap	79.53	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.371		Crippen Method
mcvol	245.530	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	814.11	K	Joback Method
tc	1022.59	K	Joback Method
tf	503.01	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.97	J/mol×K	814.11	Joback Method
cpg	759.51	J/mol×K	987.84	Joback Method
cpg	750.18	J/mol×K	953.09	Joback Method
cpg	739.75	J/mol×K	918.35	Joback Method
cpg	728.24	J/mol×K	883.60	Joback Method
cpg	715.64	J/mol×K	848.86	Joback Method
cpg	767.76	J/mol×K	1022.59	Joback Method
dvisc	0.0000579	Pa×s	814.11	Joback Method

dvisc	0.0000733	Pa×s	762.26	Joback Method
dvisc	0.0000960	Pa×s	710.41	Joback Method
dvisc	0.0001312	Pa×s	658.56	Joback Method
dvisc	0.0001890	Pa×s	606.71	Joback Method
dvisc	0.0002916	Pa×s	554.86	Joback Method
dvisc	0.0004921	Pa×s	503.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380847&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