

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

Inchi:	InChI=1S/C16H21ClO5/c1-3-4-9-21-15(18)7-8-16(19)22-11-12-5-6-13(17)10-14(12)20-21
InchiKey:	HBOJYWZUNIFTTN-UHFFFAOYSA-N
Formula:	C16H21ClO5
SMILES:	CCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	328.79

Physical Properties

Property code	Value	Unit	Source
gf	-407.78	kJ/mol	Joback Method
hf	-797.54	kJ/mol	Joback Method
hfus	41.42	kJ/mol	Joback Method
hvap	79.92	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.515		Crippen Method
mvol	245.530	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	814.55	K	Joback Method
tc	1020.52	K	Joback Method
tf	518.01	K	Joback Method
vc	0.939	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.40	J/molxK	814.55	Joback Method
cpg	714.92	J/molxK	848.88	Joback Method
cpg	727.39	J/molxK	883.21	Joback Method
cpg	738.82	J/molxK	917.53	Joback Method
cpg	749.20	J/molxK	951.86	Joback Method
cpg	758.53	J/molxK	986.19	Joback Method
cpg	766.80	J/molxK	1020.52	Joback Method
dvisc	0.0004448	Paxs	518.01	Joback Method

dvisc	0.0002788	Paxs	567.43	Joback Method
dvisc	0.0001883	Paxs	616.86	Joback Method
dvisc	0.0001348	Paxs	666.28	Joback Method
dvisc	0.0001011	Paxs	715.70	Joback Method
dvisc	0.0000787	Paxs	765.13	Joback Method
dvisc	0.0000631	Paxs	814.55	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=U380848&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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