

Succinic acid, 5-bromo-2-methoxybenzyl ethyl ester

Inchi:	InChI=1S/C14H17BrO5/c1-3-19-13(16)6-7-14(17)20-9-10-8-11(15)4-5-12(10)18-2/h4-5,8
InchiKey:	SKYZUSUQRHAYQL-UHFFFAOYSA-N
Formula:	C14H17BrO5
SMILES:	CCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC
Mol. weight [g/mol]:	345.19

Physical Properties

Property code	Value	Unit	Source
gf	-398.37	kJ/mol	Joback Method
hf	-714.19	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	77.52	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.844		Crippen Method
mvol	222.610	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2258.00		NIST Webbook
rinpol	2258.00		NIST Webbook
tb	797.52	K	Joback Method
tc	1012.86	K	Joback Method
tf	525.35	K	Joback Method
vc	0.840	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.37	J/molxK	797.52	Joback Method
cpg	654.68	J/molxK	976.97	Joback Method
cpg	646.19	J/molxK	941.08	Joback Method
cpg	636.71	J/molxK	905.19	Joback Method
cpg	626.24	J/molxK	869.30	Joback Method
cpg	614.80	J/molxK	833.41	Joback Method
cpg	662.17	J/molxK	1012.86	Joback Method
dvisc	0.0000772	Paxs	797.52	Joback Method

dvisc	0.0000948	Paxs	752.16	Joback Method
dvisc	0.0001193	Paxs	706.80	Joback Method
dvisc	0.0001551	Paxs	661.43	Joback Method
dvisc	0.0002096	Paxs	616.07	Joback Method
dvisc	0.0002970	Paxs	570.71	Joback Method
dvisc	0.0004471	Paxs	525.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381069&Units=SI

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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