

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

Inchi:	InChI=1S/C19H27BrO5/c1-3-4-5-6-7-12-24-18(21)10-11-19(22)25-14-15-13-16(20)8-9-1
InchiKey:	XSJPKAPAYBWRJH-UHFFFAOYSA-N
Formula:	C19H27BrO5
SMILES:	CCCCCCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC
Mol. weight [g/mol]:	415.32

Physical Properties

Property code	Value	Unit	Source
gf	-356.27	kJ/mol	Joback Method
hf	-817.39	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.795		Crippen Method
mcvol	293.060	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	2749.00		NIST Webbook
rinpol	2749.00		NIST Webbook
tb	911.92	K	Joback Method
tc	1124.61	K	Joback Method
tf	581.70	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.11	J/molxK	911.92	Joback Method
cpg	941.79	J/molxK	1089.16	Joback Method
cpg	933.06	J/molxK	1053.71	Joback Method
cpg	923.14	J/molxK	1018.26	Joback Method
cpg	912.01	J/molxK	982.82	Joback Method
cpg	899.67	J/molxK	947.37	Joback Method
cpg	949.34	J/molxK	1124.61	Joback Method
dvisc	0.0000376	Paxs	911.92	Joback Method

dvisc	0.0000471	Paxs	856.88	Joback Method
dvisc	0.0000607	Paxs	801.85	Joback Method
dvisc	0.0000812	Paxs	746.81	Joback Method
dvisc	0.0001139	Paxs	691.77	Joback Method
dvisc	0.0001694	Paxs	636.74	Joback Method
dvisc	0.0002714	Paxs	581.70	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=U381075&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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