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

Inchi: InChI=1S/C18H25BrO5/c1-3-4-5-6-11-23-17(20)9-10-18(21)24-13-14-12-15(19)7-8-16(14

InchiKey: TZKDLLLHWKWELM-UHFFFAOYSA-N

Formula: C18H25BrO5

SMILES: CCCCCCOC(=O)CCC(=O)OCc1cc(Br)ccc1OC

Mol. weight [g/mol]: 401.29

Physical Properties

Property code	Value	Unit	Source
gf	-364.69	kJ/mol	Joback Method
hf	-796.75	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.405		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2646.00		NIST Webbook
rinpol	2646.00		NIST Webbook
tb	889.04	K	Joback Method
tc	1100.83	K	Joback Method
tf	570.43	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.78	J/mol×K	889.04	Joback Method
cpg	841.18	J/mol×K	924.34	Joback Method
cpg	853.41	J/mol×K	959.64	Joback Method
cpg	864.47	J/mol×K	994.93	Joback Method
cpg	874.39	J/mol×K	1030.23	Joback Method
cpg	883.16	J/mol×K	1065.53	Joback Method
cpg	890.78	J/mol×K	1100.83	Joback Method
dvisc	0.0003022	Pa×s	570.43	Joback Method

dvisc	0.0001908	Pa×s	623.53	Joback Method
dvisc	0.0001295	Pa×s	676.63	Joback Method
dvisc	0.0000930	Pa×s	729.74	Joback Method
dvisc	0.0000698	Pa×s	782.84	Joback Method
dvisc	0.0000544	Pa×s	835.94	Joback Method
dvisc	0.0000437	Pa×s	889.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381074&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