Succinic acid, hept-2-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C18H25BrO5/c1-4-5-6-7-13(2)23-17(20)10-11-18(21)24-15-9-8-14(19)12-16(15

InchiKey: WSRGBGZZOIWFCW-UHFFFAOYSA-N

Formula: C18H25BrO5

SMILES: CCCCCC(C)OC(=O)CCC(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 401.29

Physical Properties

Property code	Value	Unit	Source
gf	-367.13	kJ/mol	Joback Method
hf	-802.03	kJ/mol	Joback Method
hfus	44.16	kJ/mol	Joback Method
hvap	86.03	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.655		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	888.60	K	Joback Method
tc	1102.27	K	Joback Method
tf	555.43	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.31	J/mol×K	888.60	Joback Method
cpg	841.79	J/mol×K	924.21	Joback Method
cpg	854.08	J/mol×K	959.82	Joback Method
cpg	865.17	J/mol×K	995.43	Joback Method
cpg	875.07	J/mol×K	1031.05	Joback Method
cpg	883.80	J/mol×K	1066.66	Joback Method
cpg	891.36	J/mol×K	1102.27	Joback Method
dvisc	0.0003273	Pa×s	555.43	Joback Method

dvisc	0.0001965	Pa×s	610.96	Joback Method
dvisc	0.0001285	Pa×s	666.49	Joback Method
dvisc	0.0000897	Pa×s	722.01	Joback Method
dvisc	0.0000659	Pa×s	777.54	Joback Method
dvisc	0.0000504	Pa×s	833.07	Joback Method
dvisc	0.0000399	Pa×s	888.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390917&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

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