Succinic acid, 3-methylbut-2-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C16H21BrO5/c1-10(2)11(3)21-15(18)7-8-16(19)22-13-6-5-12(17)9-14(13)20-4/

InchiKey: XPVWQJCZIVMHEZ-UHFFFAOYSA-N

Formula: C16H21BrO5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 373.24

Physical Properties

Property code	Value	Unit	Source
gf	-386.41	kJ/mol	Joback Method
hf	-766.03	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.731		Crippen Method
mcvol	250.790	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	842.40	K	Joback Method
tc	1059.87	K	Joback Method
tf	517.89	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.48	J/mol×K	842.40	Joback Method
cpg	727.76	J/mol×K	878.65	Joback Method
cpg	739.88	J/mol×K	914.89	Joback Method
cpg	750.87	J/mol×K	951.14	Joback Method
cpg	760.70	J/mol×K	987.38	Joback Method
cpg	769.40	J/mol×K	1023.63	Joback Method
cpg	776.96	J/mol×K	1059.87	Joback Method
dvisc	0.0004453	Pa×s	517.89	Joback Method

dvisc	0.0002590	Pa×s	571.98	Joback Method
dvisc	0.0001655	Pa×s	626.06	Joback Method
dvisc	0.0001135	Pa×s	680.14	Joback Method
dvisc	0.0000823	Pa×s	734.23	Joback Method
dvisc	0.0000624	Pa×s	788.31	Joback Method
dvisc	0.0000490	Pa×s	842.40	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=U390912&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