Succinic acid, 3-methylbut-2-en-1-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C16H19BrO5/c1-11(2)8-9-21-15(18)6-7-16(19)22-13-5-4-12(17)10-14(13)20-3/

InchiKey: PPRZUHPXGAGWLL-UHFFFAOYSA-N

Formula: C16H19BrO5

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

Mol. weight [g/mol]: 371.22

Physical Properties

Property code	Value	Unit	Source
gf	-309.86	kJ/mol	Joback Method
hf	-648.04	kJ/mol	Joback Method
hfus	41.40	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.653		Crippen Method
mcvol	246.490	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	847.32	K	Joback Method
tc	1067.43	K	Joback Method
tf	528.85	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.01	J/mol×K	847.32	Joback Method
cpg	698.65	J/mol×K	884.01	Joback Method
cpg	710.27	J/mol×K	920.69	Joback Method
cpg	720.87	J/mol×K	957.38	Joback Method
cpg	730.47	J/mol×K	994.06	Joback Method
cpg	739.09	J/mol×K	1030.75	Joback Method
cpg	746.75	J/mol×K	1067.43	Joback Method

Sources

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=U390914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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