Glutaric acid, 2-methylpent-3-yl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C18H25BrO5/c1-5-14(12(2)3)23-17(20)7-6-8-18(21)24-15-10-9-13(19)11-16(15

InchiKey: DIBPMOUNBJBMIX-UHFFFAOYSA-N

Formula: C18H25BrO5

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

Mol. weight [g/mol]: 401.29

Physical Properties

Property code	Value	Unit	Source
gf	-369.57	kJ/mol	Joback Method
hf	-807.31	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.511		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	888.16	K	Joback Method
tc	1103.86	K	Joback Method
tf	540.43	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.83	J/mol×K	888.16	Joback Method
cpg	884.47	J/mol×K	1067.91	Joback Method
cpg	875.78	J/mol×K	1031.96	Joback Method
cpg	865.89	J/mol×K	996.01	Joback Method
cpg	854.77	J/mol×K	960.06	Joback Method
cpg	842.42	J/mol×K	924.11	Joback Method
cpg	891.95	J/mol×K	1103.86	Joback Method
dvisc	0.0000365	Pa×s	888.16	Joback Method

dvisc	0.0000468	Pa×s	830.20	Joback Method
dvisc	0.0000622	Pa×s	772.25	Joback Method
dvisc	0.0000866	Pa×s	714.29	Joback Method
dvisc	0.0001279	Pa×s	656.34	Joback Method
dvisc	0.0002038	Pa×s	598.38	Joback Method
dvisc	0.0003588	Pa×s	540.43	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=U393883&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