Diethylmalonic acid, 3-bromobenzyl isobutyl ester

Inchi: InChI=1S/C18H25BrO4/c1-5-18(6-2,16(20)22-11-13(3)4)17(21)23-12-14-8-7-9-15(19)10-

InchiKey: TWRQYNBUNORYQB-UHFFFAOYSA-N

Formula: C18H25BrO4

SMILES: CCC(CC)(C(=O)OCc1cccc(Br)c1)C(=O)OCC(C)C

Mol. weight [g/mol]: 385.29

Physical Properties

Property code	Value	Unit	Source
gf	-249.66	kJ/mol	Joback Method
hf	-667.09	kJ/mol	Joback Method
hfus	35.95	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.498		Crippen Method
mcvol	273.100	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	857.97	K	Joback Method
tc	1077.41	K	Joback Method
tf	523.10	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.91	J/mol×K	857.97	Joback Method
cpg	817.25	J/mol×K	894.54	Joback Method
cpg	830.48	J/mol×K	931.12	Joback Method
cpg	842.63	J/mol×K	967.69	Joback Method
cpg	853.76	J/mol×K	1004.26	Joback Method
cpg	863.93	J/mol×K	1040.83	Joback Method
cpg	873.19	J/mol×K	1077.41	Joback Method
dvisc	0.0004828	Pa×s	523.10	Joback Method

dvisc	0.0002634	Pa×s	578.91	Joback Method
dvisc	0.0001599	Pa×s	634.72	Joback Method
dvisc	0.0001052	Pa×s	690.53	Joback Method
dvisc	0.0000737	Pa×s	746.35	Joback Method
dvisc	0.0000542	Pa×s	802.16	Joback Method
dvisc	0.0000415	Pa×s	857.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368411&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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