Diethylmalonic acid, 3-bromobenzyl ethyl ester

Inchi: InChI=1S/C16H21BrO4/c1-4-16(5-2,14(18)20-6-3)15(19)21-11-12-8-7-9-13(17)10-12/h7-

InchiKey: TYZBDMNGIOTRJW-UHFFFAOYSA-N

Formula: C16H21BrO4

SMILES: CCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Br)c1

Mol. weight [g/mol]: 357.24

Physical Properties

Property code	Value	Unit	Source
gf	-264.06	kJ/mol	Joback Method
hf	-620.53	kJ/mol	Joback Method
hfus	34.29	kJ/mol	Joback Method
hvap	77.60	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.862		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	812.65	K	Joback Method
tc	1033.03	K	Joback Method
tf	515.56	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.25	J/mol×K	812.65	Joback Method
cpg	702.99	J/mol×K	849.38	Joback Method
cpg	715.67	J/mol×K	886.11	Joback Method
cpg	727.35	J/mol×K	922.84	Joback Method
cpg	738.06	J/mol×K	959.57	Joback Method
cpg	747.86	J/mol×K	996.30	Joback Method
cpg	756.78	J/mol×K	1033.03	Joback Method
dvisc	0.0005387	Pa×s	515.56	Joback Method

dvisc	0.0003202	Pa×s	565.07	Joback Method
dvisc	0.0002070	Pa×s	614.59	Joback Method
dvisc	0.0001428	Pa×s	664.11	Joback Method
dvisc	0.0001037	Pa×s	713.62	Joback Method
dvisc	0.0000785	Pa×s	763.13	Joback Method
dvisc	0.0000615	Pa×s	812.65	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=U368409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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