

Malonic acid, beta-bromophenethyl-, diethyl ester

Inchi:	InChI=1S/C15H19BrO4/c1-3-19-14(17)12(15(18)20-4-2)10-13(16)11-8-6-5-7-9-11/h5-9,1
InchiKey:	QNUOOZOJYQNGMC-UHFFFAOYSA-N
Formula:	C15H19BrO4
SMILES:	CCOC(=O)C(CC(Br)c1ccccc1)C(=O)OCC
Mol. weight [g/mol]:	343.21
CAS:	116400-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-270.57	kJ/mol	Joback Method
hf	-590.23	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	75.23	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.255		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
tb	787.14	K	Joback Method
tc	1006.59	K	Joback Method
tf	459.35	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.52	J/molxK	787.14	Joback Method
cpg	648.23	J/molxK	823.72	Joback Method
cpg	660.87	J/molxK	860.29	Joback Method
cpg	672.48	J/molxK	896.87	Joback Method
cpg	683.07	J/molxK	933.44	Joback Method
cpg	692.68	J/molxK	970.02	Joback Method
cpg	701.34	J/molxK	1006.59	Joback Method
dvisc	0.0009867	Paxs	459.35	Joback Method
dvisc	0.0005099	Paxs	513.98	Joback Method

dvisc	0.0002991	Paxs	568.61	Joback Method
dvisc	0.0001927	Paxs	623.25	Joback Method
dvisc	0.0001332	Paxs	677.88	Joback Method
dvisc	0.0000973	Paxs	732.51	Joback Method
dvisc	0.0000743	Paxs	787.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116400670&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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