

Diethylmalonic acid, 4-bromo-2-methoxyphenyl butyl ester

Inchi:	InChI=1S/C18H25BrO5/c1-5-8-11-23-16(20)18(6-2,7-3)17(21)24-14-10-9-13(19)12-15(14)
InchiKey:	ZRGUYGABDZCZNP-UHFFFAOYSA-N
Formula:	C18H25BrO5
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC
Mol. weight [g/mol]:	401.29

Physical Properties

Property code	Value	Unit	Source
gf	-361.85	kJ/mol	Joback Method
hf	-805.50	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	85.12	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.513		Crippen Method
mcvol	278.970	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	2356.00		NIST Webbook
tb	885.81	K	Joback Method
tc	1103.19	K	Joback Method
tf	572.85	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.66	J/molxK	885.81	Joback Method
cpg	842.20	J/molxK	922.04	Joback Method
cpg	854.58	J/molxK	958.27	Joback Method
cpg	865.83	J/molxK	994.50	Joback Method
cpg	875.97	J/molxK	1030.73	Joback Method
cpg	885.03	J/molxK	1066.96	Joback Method
cpg	893.06	J/molxK	1103.19	Joback Method
dvisc	0.0002635	Paxs	572.85	Joback Method
dvisc	0.0001625	Paxs	625.01	Joback Method

dvisc	0.0001079	Paxs	677.17	Joback Method
dvisc	0.0000760	Paxs	729.33	Joback Method
dvisc	0.0000561	Paxs	781.49	Joback Method
dvisc	0.0000430	Paxs	833.65	Joback Method
dvisc	0.0000340	Paxs	885.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U370942&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

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