

Diethylmalonic acid, 4-bromophenyl hexyl ester

Inchi:	InChI=1S/C19H27BrO4/c1-4-7-8-9-14-23-17(21)19(5-2,6-3)18(22)24-16-12-10-15(20)11-
InchiKey:	LGSNJGBXHPXYKI-UHFFFAOYSA-N
Formula:	C19H27BrO4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	399.32

Physical Properties

Property code	Value	Unit	Source
gf	-238.80	kJ/mol	Joback Method
hf	-682.45	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	84.28	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.284		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinsol	2380.00		NIST Webbook
rinsol	2380.00		NIST Webbook
tb	881.29	K	Joback Method
tc	1097.30	K	Joback Method
tf	549.37	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.19	J/molxK	881.29	Joback Method
cpg	874.58	J/molxK	917.29	Joback Method
cpg	887.87	J/molxK	953.29	Joback Method
cpg	900.12	J/molxK	989.30	Joback Method
cpg	911.37	J/molxK	1025.30	Joback Method
cpg	921.69	J/molxK	1061.30	Joback Method
cpg	931.13	J/molxK	1097.30	Joback Method
dvisc	0.0003847	Paxs	549.37	Joback Method

dvisc	0.0002204	Paxs	604.69	Joback Method
dvisc	0.0001387	Paxs	660.01	Joback Method
dvisc	0.0000937	Paxs	715.33	Joback Method
dvisc	0.0000670	Paxs	770.65	Joback Method
dvisc	0.0000501	Paxs	825.97	Joback Method
dvisc	0.0000389	Paxs	881.29	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=U369825&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

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