Diethylmalonic acid, 4-bromophenyl pentyl ester

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

InchiKey: SFBRBTXSUMBONR-UHFFFAOYSA-N

Formula: C18H25BrO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 385.29

Physical Properties

Property code	Value	Unit	Source
gf	-247.22	kJ/mol	Joback Method
hf	-661.81	kJ/mol	Joback Method
hfus	39.47	kJ/mol	Joback Method
hvap	82.05	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.894		Crippen Method
mcvol	273.100	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2287.00		NIST Webbook
tb	858.41	K	Joback Method
tc	1075.21	K	Joback Method
tf	538.10	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.37	J/mol×K	858.41	Joback Method
cpg	816.56	J/mol×K	894.54	Joback Method
cpg	829.67	J/mol×K	930.68	Joback Method
cpg	841.75	J/mol×K	966.81	Joback Method
cpg	852.84	J/mol×K	1002.94	Joback Method
cpg	863.01	J/mol×K	1039.08	Joback Method
cpg	872.30	J/mol×K	1075.21	Joback Method
dvisc	0.0004319	Pa×s	538.10	Joback Method
dvisc	0.0002504	Pa×s	591.49	Joback Method

dvisc	0.0001589	Pa×s	644.87	Joback Method
dvisc	0.0001081	Pa×s	698.25	Joback Method
dvisc	0.0000777	Pa×s	751.64	Joback Method
dvisc	0.0000583	Pa×s	805.02	Joback Method
dvisc	0.0000454	Pa×s	858.41	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=U369824&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