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

Inchi: InChI=1S/C19H27BrO5/c1-5-8-9-12-24-17(21)19(6-2,7-3)18(22)25-15-11-10-14(20)13-16

InchiKey: NEKOTBFAMMLUQK-UHFFFAOYSA-N

Formula: C19H27BrO5

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 415.32

Physical Properties

Property code	Value	Unit	Source
gf	-353.43	kJ/mol	Joback Method
hf	-826.14	kJ/mol	Joback Method
hfus	42.86	kJ/mol	Joback Method
hvap	87.35	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.903		Crippen Method
mcvol	293.060	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	2448.00		NIST Webbook
tb	908.69	K	Joback Method
tc	1125.95	K	Joback Method
tf	584.12	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.78	J/mol×K	908.69	Joback Method
cpg	900.47	J/mol×K	944.90	Joback Method
cpg	912.97	J/mol×K	981.11	Joback Method
cpg	924.30	J/mol×K	1017.32	Joback Method
cpg	934.51	J/mol×K	1053.53	Joback Method
cpg	943.61	J/mol×K	1089.74	Joback Method
cpg	951.65	J/mol×K	1125.95	Joback Method
dvisc	0.0002348	Pa×s	584.12	Joback Method
dvisc	0.0001431	Pa×s	638.22	Joback Method

dvisc	0.0000942	Pa×s	692.31	Joback Method
dvisc	0.0000659	Pa×s	746.40	Joback Method
dvisc	0.0000484	Pa×s	800.50	Joback Method
dvisc	0.0000369	Pa×s	854.60	Joback Method
dvisc	0.0000291	Pa×s	908.69	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370947&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