Diethylmalonic acid, 4-bromophenyl butyl ester

Inchi: InChI=1S/C17H23BrO4/c1-4-7-12-21-15(19)17(5-2,6-3)16(20)22-14-10-8-13(18)9-11-14/

InchiKey: WQCRMYZNGQOHJX-UHFFFAOYSA-N

Formula: C17H23BrO4

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

Mol. weight [g/mol]: 371.27

Physical Properties

Property code	Value	Unit	Source
gf	-255.64	kJ/mol	Joback Method
hf	-641.17	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.504		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	835.53	K	Joback Method
tc	1053.80	K	Joback Method
tf	526.83	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.36	J/mol×K	835.53	Joback Method
cpg	759.34	J/mol×K	871.91	Joback Method
cpg	772.26	J/mol×K	908.29	Joback Method
cpg	784.15	J/mol×K	944.66	Joback Method
cpg	795.06	J/mol×K	981.04	Joback Method
cpg	805.06	J/mol×K	1017.42	Joback Method
cpg	814.18	J/mol×K	1053.80	Joback Method
dvisc	0.0004832	Pa×s	526.83	Joback Method

dvisc	0.0002836	Pa×s	578.28	Joback Method
dvisc	0.0001816	Pa×s	629.73	Joback Method
dvisc	0.0001244	Pa×s	681.18	Joback Method
dvisc	0.0000898	Pa×s	732.63	Joback Method
dvisc	0.0000677	Pa×s	784.08	Joback Method
dvisc	0.0000529	Pa×s	835.53	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=U369823&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