Diethylmalonic acid, di(4-bromophenyl) ester

Inchi: InChI=1S/C19H18Br2O4/c1-3-19(4-2,17(22)24-15-9-5-13(20)6-10-15)18(23)25-16-11-7-1
InchiKey: VESLXVWAXROJTR-UHFFFAOYSA-N
Formula: C19H18Br2O4
SMILES: CCC(CC)(C(=O)Oc1ccc(Br)cc1)C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 470.15

Physical Properties

Property code	Value	Unit	Source
gf	-121.70	kJ/mol	Joback Method
hf	-431.06	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	93.65	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.529		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	2868.00		NIST Webbook
rinpol	2868.00		NIST Webbook
tb	979.11	K	Joback Method
tc	1233.03	K	Joback Method
tf	648.11	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.70	J/mol×K	979.11	Joback Method
cpg	796.31	J/mol×K	1021.43	Joback Method
cpg	805.87	J/mol×K	1063.75	Joback Method
cpg	814.48	J/mol×K	1106.07	Joback Method
cpg	822.25	J/mol×K	1148.39	Joback Method
cpg	829.29	J/mol×K	1190.71	Joback Method
cpg	835.69	J/mol×K	1233.03	Joback Method
dvisc	0.0001988	Pa×s	648.11	Joback Method

dvisc	0.0001284	Pa×s	703.28	Joback Method
dvisc	0.0000884	Pa×s	758.44	Joback Method
dvisc	0.0000640	Pa×s	813.61	Joback Method
dvisc	0.0000483	Pa×s	868.78	Joback Method
dvisc	0.0000377	Pa×s	923.94	Joback Method
dvisc	0.0000302	Pa×s	979.11	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=U369835&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