Diethylmalonic acid, 3-bromobenzyl pentyl ester

Inchi: InChI=1S/C19H27BrO4/c1-4-7-8-12-23-17(21)19(5-2,6-3)18(22)24-14-15-10-9-11-16(20)

InchiKey: COYLCBQWRSRLMJ-UHFFFAOYSA-N

Formula: C19H27BrO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Br)c1

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	-6.02		Crippen Method
logp	5.032		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	881.29	K	Joback Method
tc	1097.30	K	Joback Method
tf	549.37	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.19	J/mol×K	881.29	Joback Method
cpg	921.69	J/mol×K	1061.30	Joback Method
cpg	911.37	J/mol×K	1025.30	Joback Method
cpg	900.12	J/mol×K	989.30	Joback Method
cpg	887.87	J/mol×K	953.29	Joback Method
cpg	874.58	J/mol×K	917.29	Joback Method
cpg	931.13	J/mol×K	1097.30	Joback Method
dvisc	0.0000389	Pa×s	881.29	Joback Method

dvisc	0.0000501	Pa×s	825.97	Joback Method
dvisc	0.0000670	Pa×s	770.65	Joback Method
dvisc	0.0000937	Pa×s	715.33	Joback Method
dvisc	0.0001387	Pa×s	660.01	Joback Method
dvisc	0.0002204	Pa×s	604.69	Joback Method
dvisc	0.0003847	Pa×s	549.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368413&Units=SI
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

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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