Diethylmalonic acid, 3-bromobenzyl nonyl ester

Inchi: InChI=1S/C23H35BrO4/c1-4-7-8-9-10-11-12-16-27-21(25)23(5-2,6-3)22(26)28-18-19-14-

InchiKey: SLMPIBBEDMOBRA-UHFFFAOYSA-N

Formula: C23H35BrO4

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

Mol. weight [g/mol]: 455.43

Physical Properties

Property code	Value	Unit	Source
gf	-205.12	kJ/mol	Joback Method
hf	-765.01	kJ/mol	Joback Method
hfus	52.42	kJ/mol	Joback Method
hvap	93.18	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.593		Crippen Method
mcvol	343.550	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
rinpol	2737.00		NIST Webbook
tb	972.81	K	Joback Method
tc	1193.48	K	Joback Method
tf	594.45	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.56	J/mol×K	972.81	Joback Method
cpg	1113.78	J/mol×K	1009.59	Joback Method
cpg	1127.79	J/mol×K	1046.37	Joback Method
cpg	1140.68	J/mol×K	1083.15	Joback Method
cpg	1152.50	J/mol×K	1119.93	Joback Method
cpg	1163.34	J/mol×K	1156.71	Joback Method
cpg	1173.27	J/mol×K	1193.48	Joback Method
dvisc	0.0002351	Pa×s	594.45	Joback Method
dvisc	0.0001290	Pa×s	657.51	Joback Method

dvisc	0.0000786	Pa×s	720.57	Joback Method
dvisc	0.0000519	Pa×s	783.63	Joback Method
dvisc	0.0000364	Pa×s	846.69	Joback Method
dvisc	0.0000269	Pa×s	909.75	Joback Method
dvisc	0.0000206	Pa×s	972.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368417&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

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