Diethylmalonic acid, 3-bromobenzyl heptadecyl ester

Inchi: InChI=1S/C31H51BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-35-29(33)31(5

InchiKey: XLCSAMJTIDVYLL-UHFFFAOYSA-N

Formula: C31H51BrO4

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

Mol. weight [g/mol]: 567.64

Physical Properties

Property code	Value	Unit	Source
gf	-137.76	kJ/mol	Joback Method
hf	-930.13	kJ/mol	Joback Method
hfus	73.14	kJ/mol	Joback Method
hvap	110.99	kJ/mol	Joback Method
log10ws	-11.04		Crippen Method
logp	9.713		Crippen Method
mcvol	456.270	ml/mol	McGowan Method
pc	731.25	kPa	Joback Method
rinpol	3376.00		NIST Webbook
rinpol	3376.00		NIST Webbook
tb	1155.85	K	Joback Method
tc	1436.32	K	Joback Method
tf	684.61	K	Joback Method
vc	1.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1599.86	J/mol×K	1155.85	Joback Method
cpg	1618.47	J/mol×K	1202.60	Joback Method
cpg	1635.35	J/mol×K	1249.34	Joback Method
cpg	1650.70	J/mol×K	1296.09	Joback Method
cpg	1664.74	J/mol×K	1342.83	Joback Method
cpg	1677.66	J/mol×K	1389.58	Joback Method
cpg	1689.68	J/mol×K	1436.32	Joback Method
dvisc	0.0000786	Pa×s	684.61	Joback Method

dvisc	0.0000401	Pa×s	763.15	Joback Method
dvisc	0.0000232	Pa×s	841.69	Joback Method
dvisc	0.0000147	Pa×s	920.23	Joback Method
dvisc	0.0000101	Pa×s	998.77	Joback Method
dvisc	0.0000073	Pa×s	1077.31	Joback Method
dvisc	0.0000055	Pa×s	1155.85	Joback Method

Sources

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=U368424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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