Diethylmalonic acid, 3-bromobenzyl octadecyl ester

Inchi: InChI=1S/C32H53BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-36-30(34)3

InchiKey: RNGARFMARSIFOE-UHFFFAOYSA-N

Formula: C32H53BrO4

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

Mol. weight [g/mol]: 581.66

Physical Properties

Property code	Value	Unit	Source
gf	-129.34	kJ/mol	Joback Method
hf	-950.77	kJ/mol	Joback Method
hfus	75.73	kJ/mol	Joback Method
hvap	113.21	kJ/mol	Joback Method
log10ws	-11.46		Crippen Method
logp	10.103		Crippen Method
mcvol	470.360	ml/mol	McGowan Method
pc	694.71	kPa	Joback Method
rinpol	3483.00		NIST Webbook
tb	1178.73	K	Joback Method
tc	1473.01	K	Joback Method
tf	695.88	K	Joback Method
vc	1.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1664.17	J/mol×K	1178.73	Joback Method
cpg	1745.00	J/mol×K	1423.97	Joback Method
cpg	1731.52	J/mol×K	1374.92	Joback Method
cpg	1716.94	J/mol×K	1325.87	Joback Method
cpg	1701.02	J/mol×K	1276.82	Joback Method
cpg	1683.51	J/mol×K	1227.78	Joback Method
cpg	1757.63	J/mol×K	1473.01	Joback Method
dvisc	0.0000046	Pa×s	1178.73	Joback Method
dvisc	0.0000061	Pa×s	1098.26	Joback Method

dvisc	0.0000085	Pa×s	1017.78	Joback Method
dvisc	0.0000125	Pa×s	937.31	Joback Method
dvisc	0.0000198	Pa×s	856.83	Joback Method
dvisc	0.0000344	Pa×s	776.36	Joback Method
dvisc	0.0000680	Pa×s	695.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368425&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