Diethylmalonic acid, 3-bromobenzyl hexadecyl ester

Inchi: InChI=1S/C30H49BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-34-28(32)30(5-2,6

InchiKey: KDDGSKYBRPPJCK-UHFFFAOYSA-N

Formula: C30H49BrO4

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

Mol. weight [g/mol]: 553.61

Physical Properties

Property code	Value	Unit	Source
gf	-146.18	kJ/mol	Joback Method
hf	-909.49	kJ/mol	Joback Method
hfus	70.55	kJ/mol	Joback Method
hvap	108.76	kJ/mol	Joback Method
log10ws	-10.62		Crippen Method
logp	9.323		Crippen Method
mcvol	442.180	ml/mol	McGowan Method
pc	770.75	kPa	Joback Method
rinpol	3293.00		NIST Webbook
rinpol	3293.00		NIST Webbook
tb	1132.97	K	Joback Method
tc	1401.28	K	Joback Method
tf	673.34	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1535.86	J/mol×K	1132.97	Joback Method
cpg	1553.82	J/mol×K	1177.69	Joback Method
cpg	1570.15	J/mol×K	1222.41	Joback Method
cpg	1585.02	J/mol×K	1267.12	Joback Method
cpg	1598.61	J/mol×K	1311.84	Joback Method
cpg	1611.08	J/mol×K	1356.56	Joback Method
cpg	1622.61	J/mol×K	1401.28	Joback Method
dvisc	0.0000907	Pa×s	673.34	Joback Method

dvisc	0.0000467	Pa×s	749.94	Joback Method
dvisc	0.0000272	Pa×s	826.55	Joback Method
dvisc	0.0000173	Pa×s	903.15	Joback Method
dvisc	0.0000119	Pa×s	979.76	Joback Method
dvisc	0.0000086	Pa×s	1056.36	Joback Method
dvisc	0.0000065	Pa×s	1132.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368423&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