Diethylmalonic acid, 3-bromobenzyl pentadecyl ester

Inchi: InChI=1S/C29H47BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-33-27(31)29(5-2,6-3)
InchiKey: KCYLXDRQBRTXLS-UHFFFAOYSA-N
Formula: C29H47BrO4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]: 539.59

Physical Properties

Property code	Value	Unit	Source
gf	-154.60	kJ/mol	Joback Method
hf	-888.85	kJ/mol	Joback Method
hfus	67.96	kJ/mol	Joback Method
hvap	106.54	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	8.933		Crippen Method
mcvol	428.090	ml/mol	McGowan Method
pc	813.53	kPa	Joback Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook
tb	1110.09	K	Joback Method
tc	1367.77	K	Joback Method
tf	662.07	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1472.19	J/mol×K	1110.09	Joback Method
cpg	1545.19	J/mol×K	1324.82	Joback Method
cpg	1533.09	J/mol×K	1281.87	Joback Method
cpg	1519.89	J/mol×K	1238.93	Joback Method
cpg	1505.44	J/mol×K	1195.98	Joback Method
cpg	1489.59	J/mol×K	1153.04	Joback Method
cpg	1556.34	J/mol×K	1367.77	Joback Method
dvisc	0.0000077	Pa×s	1110.09	Joback Method

dvisc	0.0000101	Pa×s	1035.42	Joback Method
dvisc	0.0000140	Pa×s	960.75	Joback Method
dvisc	0.0000204	Pa×s	886.08	Joback Method
dvisc	0.0000318	Pa×s	811.41	Joback Method
dvisc	0.0000543	Pa×s	736.74	Joback Method
dvisc	0.0001045	Pa×s	662.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368422&Units=SI

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