Diethylmalonic acid, 3-bromobenzyl tetradecyl ester

Inchi: InChI=1S/C28H45BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-32-26(30)28(5-2,6-3)27(

InchiKey: KNZUEVSDWBEOFF-UHFFFAOYSA-N

Formula: C28H45BrO4

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

Mol. weight [g/mol]: 525.56

Physical Properties

Property code	Value	Unit	Source
gf	-163.02	kJ/mol	Joback Method
hf	-868.21	kJ/mol	Joback Method
hfus	65.37	kJ/mol	Joback Method
hvap	104.31	kJ/mol	Joback Method
log10ws	-9.79		Crippen Method
logp	8.543		Crippen Method
mcvol	414.000	ml/mol	McGowan Method
pc	859.99	kPa	Joback Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		NIST Webbook
tb	1087.21	K	Joback Method
tc	1335.68	K	Joback Method
tf	650.80	K	Joback Method
vc	1.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1408.87	J/mol×K	1087.21	Joback Method
cpg	1479.97	J/mol×K	1294.27	Joback Method
cpg	1468.18	J/mol×K	1252.86	Joback Method
cpg	1455.30	J/mol×K	1211.44	Joback Method
cpg	1441.20	J/mol×K	1170.03	Joback Method
cpg	1425.77	J/mol×K	1128.62	Joback Method
cpg	1490.81	J/mol×K	1335.68	Joback Method
dvisc	0.0000091	Pa×s	1087.21	Joback Method

dvisc	0.0000120	Pa×s	1014.48	Joback Method
dvisc	0.0000164	Pa×s	941.74	Joback Method
dvisc	0.0000239	Pa×s	869.00	Joback Method
dvisc	0.0000371	Pa×s	796.27	Joback Method
dvisc	0.0000629	Pa×s	723.53	Joback Method
dvisc	0.0001203	Pa×s	650.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368421&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