Diethylmalonic acid, 3-bromobenzyl tridecyl ester

Inchi: InChI=1S/C27H43BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-20-31-25(29)27(5-2,6-3)26(30)
InchiKey: WJGDAYOKFGPKED-UHFFFAOYSA-N
Formula: C27H43BrO4
SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]: 511.53

Physical Properties

Property code	Value	Unit	Source
gf	-171.44	kJ/mol	Joback Method
hf	-847.57	kJ/mol	Joback Method
hfus	62.78	kJ/mol	Joback Method
hvap	102.08	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.153		Crippen Method
mcvol	399.910	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
rinpol	3102.00		NIST Webbook
rinpol	3102.00		NIST Webbook
tb	1064.33	K	Joback Method
tc	1304.92	K	Joback Method
tf	639.53	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.92	J/mol×K	1064.33	Joback Method
cpg	1362.39	J/mol×K	1104.43	Joback Method
cpg	1377.46	J/mol×K	1144.53	Joback Method
cpg	1391.24	J/mol×K	1184.62	Joback Method
cpg	1403.85	J/mol×K	1224.72	Joback Method
cpg	1415.39	J/mol×K	1264.82	Joback Method
cpg	1425.98	J/mol×K	1304.92	Joback Method
dvisc	0.0001381	Pa×s	639.53	Joback Method

dvisc	0.0000729	Pa×s	710.33	Joback Method
dvisc	0.0000432	Pa×s	781.13	Joback Method
dvisc	0.0000280	Pa×s	851.93	Joback Method
dvisc	0.0000193	Pa×s	922.73	Joback Method
dvisc	0.0000141	Pa×s	993.53	Joback Method
dvisc	0.0000107	Pa×s	1064.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368420&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

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