Diethylmalonic acid, 3-bromobenzyl octyl ester

Inchi: InChI=1S/C22H33BrO4/c1-4-7-8-9-10-11-15-26-20(24)22(5-2,6-3)21(25)27-17-18-13-12-

InchiKey: CBVGJPKZAYYBCG-UHFFFAOYSA-N

Formula: C22H33BrO4

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

Mol. weight [g/mol]: 441.40

Physical Properties

Property code	Value	Unit	Source
gf	-213.54	kJ/mol	Joback Method
hf	-744.37	kJ/mol	Joback Method
hfus	49.83	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.202		Crippen Method
mcvol	329.460	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook
tb	949.93	K	Joback Method
tc	1168.16	K	Joback Method
tf	583.18	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.02	J/mol×K	949.93	Joback Method
cpg	1101.92	J/mol×K	1131.79	Joback Method
cpg	1091.21	J/mol×K	1095.42	Joback Method
cpg	1079.54	J/mol×K	1059.05	Joback Method
cpg	1066.82	J/mol×K	1022.67	Joback Method
cpg	1053.00	J/mol×K	986.30	Joback Method
cpg	1111.73	J/mol×K	1168.16	Joback Method
dvisc	0.0000242	Pa×s	949.93	Joback Method

dvisc	0.0000315	Pa×s	888.80	Joback Method
dvisc	0.0000425	Pa×s	827.68	Joback Method
dvisc	0.0000603	Pa×s	766.56	Joback Method
dvisc	0.0000909	Pa×s	705.43	Joback Method
dvisc	0.0001480	Pa×s	644.31	Joback Method
dvisc	0.0002670	Pa×s	583.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368416&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