Diethylmalonic acid, 3-bromobenzyl decyl ester

Inchi: InChI=1S/C24H37BrO4/c1-4-7-8-9-10-11-12-13-17-28-22(26)24(5-2,6-3)23(27)29-19-20-

InchiKey: AXRKPBAYFQYRAT-UHFFFAOYSA-N

Formula: C24H37BrO4

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

Mol. weight [g/mol]: 469.45

Physical Properties

Property code	Value	Unit	Source
gf	-196.70	kJ/mol	Joback Method
hf	-785.65	kJ/mol	Joback Method
hfus	55.01	kJ/mol	Joback Method
hvap	95.41	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.983		Crippen Method
mcvol	357.640	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	995.69	K	Joback Method
tc	1219.75	K	Joback Method
tf	605.72	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.67	J/mol×K	995.69	Joback Method
cpg	1175.14	J/mol×K	1033.03	Joback Method
cpg	1189.37	J/mol×K	1070.38	Joback Method
cpg	1202.44	J/mol×K	1107.72	Joback Method
cpg	1214.42	J/mol×K	1145.07	Joback Method
cpg	1225.41	J/mol×K	1182.41	Joback Method
cpg	1235.47	J/mol×K	1219.75	Joback Method
dvisc	0.0002065	Pa×s	605.72	Joback Method

dvisc	0.0001122	Pa×s	670.72	Joback Method
dvisc	0.0000679	Pa×s	735.71	Joback Method
dvisc	0.0000446	Pa×s	800.70	Joback Method
dvisc	0.0000312	Pa×s	865.70	Joback Method
dvisc	0.0000229	Pa×s	930.69	Joback Method
dvisc	0.0000175	Pa×s	995.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368418&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