Diethylmalonic acid, 3-bromobenzyl hexyl ester

Inchi: InChI=1S/C20H29BrO4/c1-4-7-8-9-13-24-18(22)20(5-2,6-3)19(23)25-15-16-11-10-12-17(

InchiKey: QGHKIYPQUNHPLX-UHFFFAOYSA-N

Formula: C20H29BrO4

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

Mol. weight [g/mol]: 413.35

Physical Properties

Property code	Value	Unit	Source
gf	-230.38	kJ/mol	Joback Method
hf	-703.09	kJ/mol	Joback Method
hfus	44.65	kJ/mol	Joback Method
hvap	86.50	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.422		Crippen Method
mcvol	301.280	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	904.17	K	Joback Method
tc	1120.13	K	Joback Method
tf	560.64	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.78	J/mol×K	904.17	Joback Method
cpg	981.08	J/mol×K	1084.14	Joback Method
cpg	970.63	J/mol×K	1048.14	Joback Method
cpg	959.23	J/mol×K	1012.15	Joback Method
cpg	946.83	J/mol×K	976.16	Joback Method
cpg	933.36	J/mol×K	940.16	Joback Method
cpg	990.65	J/mol×K	1120.13	Joback Method
dvisc	0.0000332	Pa×s	904.17	Joback Method

dvisc	0.0000430	Pa×s	846.91	Joback Method
dvisc	0.0000577	Pa×s	789.66	Joback Method
dvisc	0.0000811	Pa×s	732.40	Joback Method
dvisc	0.0001207	Pa×s	675.15	Joback Method
dvisc	0.0001935	Pa×s	617.89	Joback Method
dvisc	0.0003416	Pa×s	560.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368414&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