Diethylmalonic acid, 4-bromo-2-methoxyphenyl heptyl ester

Inchi: InChI=1S/C21H31BrO5/c1-5-8-9-10-11-14-26-19(23)21(6-2,7-3)20(24)27-17-13-12-16(22

InchiKey: QWDVFMQFYJNLFO-UHFFFAOYSA-N

Formula: C21H31BrO5

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 443.37

Physical Properties

Property code	Value	Unit	Source
gf	-336.59	kJ/mol	Joback Method
hf	-867.42	kJ/mol	Joback Method
hfus	48.04	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.683		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	954.45	K	Joback Method
tc	1173.86	K	Joback Method
tf	606.66	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.99	J/mol×K	954.45	Joback Method
cpg	1018.97	J/mol×K	991.02	Joback Method
cpg	1031.67	J/mol×K	1027.59	Joback Method
cpg	1043.14	J/mol×K	1064.16	Joback Method
cpg	1053.40	J/mol×K	1100.72	Joback Method
cpg	1062.51	J/mol×K	1137.29	Joback Method
cpg	1070.49	J/mol×K	1173.86	Joback Method
dvisc	0.0001848	Pa×s	606.66	Joback Method

dvisc	0.0001101	Pa×s	664.62	Joback Method
dvisc	0.0000713	Pa×s	722.59	Joback Method
dvisc	0.0000492	Pa×s	780.56	Joback Method
dvisc	0.0000358	Pa×s	838.52	Joback Method
dvisc	0.0000271	Pa×s	896.49	Joback Method
dvisc	0.0000212	Pa×s	954.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370951&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