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

Inchi: InChI=1S/C22H33BrO5/c1-5-8-9-10-11-12-15-27-20(24)22(6-2,7-3)21(25)28-18-14-13-17

InchiKey: UZHKNCVEXQNSFV-UHFFFAOYSA-N

Formula: C22H33BrO5

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

Mol. weight [g/mol]: 457.40

Physical Properties

Property code	Value	Unit	Source
gf	-328.17	kJ/mol	Joback Method
hf	-888.06	kJ/mol	Joback Method
hfus	50.63	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.073		Crippen Method
mcvol	335.330	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2727.00		NIST Webbook
tb	977.33	K	Joback Method
tc	1199.13	K	Joback Method
tf	617.93	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.97	J/mol×K	977.33	Joback Method
cpg	1079.10	J/mol×K	1014.30	Joback Method
cpg	1091.90	J/mol×K	1051.26	Joback Method
cpg	1103.41	J/mol×K	1088.23	Joback Method
cpg	1113.68	J/mol×K	1125.20	Joback Method
cpg	1122.76	J/mol×K	1162.16	Joback Method
cpg	1130.69	J/mol×K	1199.13	Joback Method
dvisc	0.0001633	Pa×s	617.93	Joback Method
dvisc	0.0000963	Pa×s	677.83	Joback Method

dvisc	0.0000618	Pa×s	737.73	Joback Method
dvisc	0.0000424	Pa×s	797.63	Joback Method
dvisc	0.0000307	Pa×s	857.53	Joback Method
dvisc	0.0000232	Pa×s	917.43	Joback Method
dvisc	0.0000181	Pa×s	977.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370952&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