Diethylmalonic acid, 4-bromo-2-methoxyphenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C21H31BrO5/c1-7-10-16(14(4)5)26-19(23)21(8-2,9-3)20(24)27-17-12-11-15(22
InchiKey: GRWOIIQZRWPPSO-UHFFFAOYSA-N
Formula: C21H31BrO5
SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1OC)C(C)C
Mol. weight [g/mol]: 443.37

Physical Properties

Property code	Value	Unit	Source
gf	-341.47	kJ/mol	Joback Method
hf	-877.98	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.537		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	953.57	K	Joback Method
tc	1175.66	K	Joback Method
tf	576.66	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.88	J/mol×K	953.57	Joback Method
cpg	1019.93	J/mol×K	990.59	Joback Method
cpg	1032.64	J/mol×K	1027.60	Joback Method
cpg	1044.05	J/mol×K	1064.62	Joback Method
cpg	1054.22	J/mol×K	1101.63	Joback Method
cpg	1063.17	J/mol×K	1138.65	Joback Method
cpg	1070.94	J/mol×K	1175.66	Joback Method
dvisc	0.0002195	Pa×s	576.66	Joback Method

dvisc	0.0001173	Pa×s	639.48	Joback Method
dvisc	0.0000701	Pa×s	702.30	Joback Method
dvisc	0.0000456	Pa×s	765.12	Joback Method
dvisc	0.0000317	Pa×s	827.93	Joback Method
dvisc	0.0000232	Pa×s	890.75	Joback Method
dvisc	0.0000176	Pa×s	953.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370933&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