Dimethylmalonic acid, 2-bromo-4-fluorophenyl nonyl ester

Inchi: InChI=1S/C20H28BrFO4/c1-4-5-6-7-8-9-10-13-25-18(23)20(2,3)19(24)26-17-12-11-15(22

InchiKey: DQGMXGIZIUYZCU-UHFFFAOYSA-N

Formula: C20H28BrFO4

SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 431.34

Physical Properties

Property code	Value	Unit	Source
gf	-434.82	kJ/mol	Joback Method
hf	-910.67	kJ/mol	Joback Method
hfus	47.34	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.814		Crippen Method
mcvol	303.050	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	908.42	K	Joback Method
tc	1121.12	K	Joback Method
tf	573.75	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.94	J/mol×K	908.42	Joback Method
cpg	939.05	J/mol×K	943.87	Joback Method
cpg	952.07	J/mol×K	979.32	Joback Method
cpg	964.06	J/mol×K	1014.77	Joback Method
cpg	975.05	J/mol×K	1050.22	Joback Method
cpg	985.10	J/mol×K	1085.67	Joback Method
cpg	994.26	J/mol×K	1121.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361826&Units=SI

Legend

cpg:	Ideal gas heat capacity
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