Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl 2-methylhex-3-yl ester

Inchi: InChI=1S/C17H28BrF3O4/c1-6-9-12(11(4)5)24-14(22)16(7-2,8-3)15(23)25-13(10-18)17(

InchiKey: FMNMGMIPRRFQGF-UHFFFAOYSA-N

Formula: C17H28BrF3O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F)C(C)C

Mol. weight [g/mol]: 433.30

Physical Properties

Property code	Value	Unit	Source
gf	-947.33	kJ/mol	Joback Method
hf	-1479.15	kJ/mol	Joback Method
hfus	34.49	kJ/mol	Joback Method
hvap	71.98	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.030		Crippen Method
mcvol	288.080	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	797.13	K	Joback Method
tc	987.69	K	Joback Method
tf	447.08	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.28	J/mol×K	797.13	Joback Method
cpg	880.35	J/mol×K	828.89	Joback Method
cpg	894.46	J/mol×K	860.65	Joback Method
cpg	907.66	J/mol×K	892.41	Joback Method
cpg	920.00	J/mol×K	924.17	Joback Method
cpg	931.52	J/mol×K	955.93	Joback Method
cpg	942.27	J/mol×K	987.69	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=U370797&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