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

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

InchiKey: PKQSHOAUWKWXEG-UHFFFAOYSA-N

Formula: C17H28BrF3O4

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

Mol. weight [g/mol]: 433.30

Physical Properties

Property code	Value	Unit	Source
gf	-942.45	kJ/mol	Joback Method
hf	-1468.59	kJ/mol	Joback Method
hfus	41.53	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.175		Crippen Method
mcvol	288.080	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	1846.00		NIST Webbook
rinpol	1846.00		NIST Webbook
tb	798.01	K	Joback Method
tc	985.52	K	Joback Method
tf	477.08	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.21	J/mol×K	798.01	Joback Method
cpg	879.04	J/mol×K	829.26	Joback Method
cpg	892.96	J/mol×K	860.51	Joback Method
cpg	906.01	J/mol×K	891.77	Joback Method
cpg	918.24	J/mol×K	923.02	Joback Method
cpg	929.70	J/mol×K	954.27	Joback Method
cpg	940.43	J/mol×K	985.52	Joback Method

Sources

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=U370799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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