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

Inchi: InChI=1S/C15H24BrF3O4/c1-4-5-6-7-8-9-22-12(20)14(2,3)13(21)23-11(10-16)15(17,18)1

InchiKey: SDNGZIJMIAAPQS-UHFFFAOYSA-N

Formula: C15H24BrF3O4

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

Mol. weight [g/mol]: 405.25

Physical Properties

Property code	Value	Unit	Source
gf	-959.29	kJ/mol	Joback Method
hf	-1427.31	kJ/mol	Joback Method
hfus	36.35	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.395		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	752.25	K	Joback Method
tc	938.03	K	Joback Method
tf	454.54	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.07	J/mol×K	752.25	Joback Method
cpg	765.16	J/mol×K	783.21	Joback Method
cpg	778.40	J/mol×K	814.18	Joback Method
cpg	790.81	J/mol×K	845.14	Joback Method
cpg	802.44	J/mol×K	876.10	Joback Method
cpg	813.33	J/mol×K	907.07	Joback Method
cpg	823.52	J/mol×K	938.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361933&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
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