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

Inchi: InChI=1S/C18H30BrF3O4/c1-4-7-8-9-10-11-12-25-15(23)17(5-2,6-3)16(24)26-14(13-19)

InchiKey: DGRUBQWADMNGID-UHFFFAOYSA-N

Formula: C18H30BrF3O4

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

Mol. weight [g/mol]: 447.33

Physical Properties

Property code	Value	Unit	Source
gf	-934.03	kJ/mol	Joback Method
hf	-1489.23	kJ/mol	Joback Method
hfus	44.12	kJ/mol	Joback Method
hvap	74.98	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.566		Crippen Method
mcvol	302.170	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
tb	820.89	K	Joback Method
tc	1010.26	K	Joback Method
tf	488.35	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.16	J/mol×K	820.89	Joback Method
cpg	937.37	J/mol×K	852.45	Joback Method
cpg	951.63	J/mol×K	884.01	Joback Method
cpg	965.00	J/mol×K	915.57	Joback Method
cpg	977.53	J/mol×K	947.14	Joback Method
cpg	989.26	J/mol×K	978.70	Joback Method
cpg	1000.25	J/mol×K	1010.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370800&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