Malonic acid, butyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H14F8O4/c1-2-3-4-23-7(21)5-8(22)24-6-10(15,16)12(19,20)11(17,18)9(13)

InchiKey: QOOYOAVOVBGFEB-UHFFFAOYSA-N

Formula: C12H14F8O4

SMILES: CCCCOC(=O)CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 374.22

Physical Properties

Property code	Value	Unit	Source
gf	-1970.08	kJ/mol	Joback Method
hf	-2381.02	kJ/mol	Joback Method
hfus	31.29	kJ/mol	Joback Method
hvap	49.81	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.434		Crippen Method
mcvol	208.980	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	1360.00		NIST Webbook
tb	610.57	K	Joback Method
tc	765.62	K	Joback Method
tf	366.30	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.05	J/mol×K	610.57	Joback Method
cpg	602.35	J/mol×K	636.41	Joback Method
cpg	613.95	J/mol×K	662.25	Joback Method
cpg	624.90	J/mol×K	688.09	Joback Method
cpg	635.21	J/mol×K	713.94	Joback Method
cpg	644.92	J/mol×K	739.78	Joback Method
cpg	654.04	J/mol×K	765.62	Joback Method

Sources

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=U349348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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