Diethylmalonic acid, butyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C15H21F7O4/c1-4-7-8-25-10(23)12(5-2,6-3)11(24)26-9-13(16,17)14(18,19)15(

InchiKey: QVGZVUXDHYKBQR-UHFFFAOYSA-N

Formula: C15H21F7O4

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

Mol. weight [g/mol]: 398.31

Physical Properties

Property code	Value	Unit	Source
gf	-1744.73	kJ/mol	Joback Method
hf	-2250.30	kJ/mol	Joback Method
hfus	32.08	kJ/mol	Joback Method
hvap	56.39	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.512		Crippen Method
mcvol	249.480	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	677.15	K	Joback Method
tc	842.12	K	Joback Method
tf	416.94	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.15	J/mol×K	677.15	Joback Method
cpg	756.25	J/mol×K	704.64	Joback Method
cpg	769.50	J/mol×K	732.14	Joback Method
cpg	781.94	J/mol×K	759.63	Joback Method
cpg	793.63	J/mol×K	787.13	Joback Method
cpg	804.61	J/mol×K	814.62	Joback Method
cpg	814.93	J/mol×K	842.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368429&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