Diethylmalonic acid, isobutyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H21F5O4/c1-5-18(6-2,16(24)26-7-9(3)4)17(25)27-8-10-11(19)13(21)15(23)

InchiKey: VUBJOQJAJWGUEA-UHFFFAOYSA-N

Formula: C18H21F5O4

SMILES: CCC(CC)(C(=O)OCc1c(F)c(F)c(F)c(F)c1F)C(=O)OCC(C)C

Mol. weight [g/mol]: 396.35

Physical Properties

Property code	Value	Unit	Source
gf	-1276.55	kJ/mol	Joback Method
hf	-1719.85	kJ/mol	Joback Method
hfus	44.51	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.431		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1752.00		NIST Webbook
tb	808.08	K	Joback Method
tc	996.46	K	Joback Method
tf	516.33	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.79	J/mol×K	808.08	Joback Method
cpg	811.32	J/mol×K	839.48	Joback Method
cpg	823.93	J/mol×K	870.87	Joback Method
cpg	835.66	J/mol×K	902.27	Joback Method
cpg	846.52	J/mol×K	933.66	Joback Method
cpg	856.51	J/mol×K	965.06	Joback Method
cpg	865.65	J/mol×K	996.46	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=U369989&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