Dimethylmalonic acid, heptyl pentafluorophenyl ester

Inchi: InChI=1S/C18H21F5O4/c1-4-5-6-7-8-9-26-16(24)18(2,3)17(25)27-15-13(22)11(20)10(19
InchiKey: LNSUIGDRSARXOR-UHFFFAOYSA-N
Formula: C18H21F5O4
SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 396.35

Physical Properties

Property code	Value	Unit	Source
gf	-1274.11	kJ/mol	Joback Method
hf	-1714.57	kJ/mol	Joback Method
hfus	48.03	kJ/mol	Joback Method
hvap	74.18	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.827		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1845.00		NIST Webbook
tb	808.52	K	Joback Method
tc	995.69	K	Joback Method
tf	531.33	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.24	J/mol×K	808.52	Joback Method
cpg	810.68	J/mol×K	839.72	Joback Method
cpg	823.23	J/mol×K	870.91	Joback Method
cpg	834.92	J/mol×K	902.11	Joback Method
cpg	845.75	J/mol×K	933.30	Joback Method
cpg	855.74	J/mol×K	964.50	Joback Method
cpg	864.90	J/mol×K	995.69	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=U363664&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