Diethylmalonic acid, heptyl pentafluorobenzyl ester

Inchi: InChI=1S/C21H27F5O4/c1-4-7-8-9-10-11-29-19(27)21(5-2,6-3)20(28)30-12-13-14(22)16
InchiKey: RQEOXXZOBALPCF-UHFFFAOYSA-N
Formula: C21H27F5O4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 438.43

Physical Properties

Property code	Value	Unit	Source
gf	-1248.85	kJ/mol	Joback Method
hf	-1776.49	kJ/mol	Joback Method
hfus	55.80	kJ/mol	Joback Method
hvap	80.86	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	5.745		Crippen Method
mcvol	306.720	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	877.16	K	Joback Method
tc	1074.10	K	Joback Method
tf	565.14	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.43	J/mol×K	877.16	Joback Method
cpg	986.11	J/mol×K	909.98	Joback Method
cpg	999.70	J/mol×K	942.81	Joback Method
cpg	1012.24	J/mol×K	975.63	Joback Method
cpg	1023.73	J/mol×K	1008.45	Joback Method
cpg	1034.21	J/mol×K	1041.27	Joback Method
cpg	1043.70	J/mol×K	1074.10	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=U369993&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