Diethylmalonic acid, hexyl pentafluorobenzyl ester

Inchi: InChI=1S/C20H25F5O4/c1-4-7-8-9-10-28-18(26)20(5-2,6-3)19(27)29-11-12-13(21)15(23

InchiKey: BQHHLPYRNGAUGX-UHFFFAOYSA-N

Formula: C20H25F5O4

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

Mol. weight [g/mol]: 424.40

Physical Properties

Property code	Value	Unit	Source
gf	-1257.27	kJ/mol	Joback Method
hf	-1755.85	kJ/mol	Joback Method
hfus	53.21	kJ/mol	Joback Method
hvap	78.63	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.355		Crippen Method
mcvol	292.630	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	854.28	K	Joback Method
tc	1047.14	K	Joback Method
tf	553.87	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.58	J/mol×K	854.28	Joback Method
cpg	926.84	J/mol×K	886.42	Joback Method
cpg	940.09	J/mol×K	918.57	Joback Method
cpg	952.35	J/mol×K	950.71	Joback Method
cpg	963.65	J/mol×K	982.85	Joback Method
cpg	973.99	J/mol×K	1015.00	Joback Method
cpg	983.40	J/mol×K	1047.14	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=U369992&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