Diethylmalonic acid, decyl pentafluorobenzyl ester

Inchi: InChI=1S/C24H33F5O4/c1-4-7-8-9-10-11-12-13-14-32-22(30)24(5-2,6-3)23(31)33-15-16
InchiKey: IHORQARQPXXXSU-UHFFFAOYSA-N
Formula: C24H33F5O4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 480.51

Physical Properties

Property code	Value	Unit	Source
gf	-1223.59	kJ/mol	Joback Method
hf	-1838.41	kJ/mol	Joback Method
hfus	63.57	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	6.916		Crippen Method
mcvol	348.990	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	945.80	K	Joback Method
tc	1160.70	K	Joback Method
tf	598.95	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.93	J/mol×K	945.80	Joback Method
cpg	1167.96	J/mol×K	981.62	Joback Method
cpg	1182.60	J/mol×K	1017.43	Joback Method
cpg	1195.91	J/mol×K	1053.25	Joback Method
cpg	1207.91	J/mol×K	1089.07	Joback Method
cpg	1218.67	J/mol×K	1124.88	Joback Method
cpg	1228.20	J/mol×K	1160.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369996&Units=SI

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