Diethylmalonic acid, 3,4-difluorobenzyl heptyl ester

Inchi: InChI=1S/C21H30F2O4/c1-4-7-8-9-10-13-26-19(24)21(5-2,6-3)20(25)27-15-16-11-12-17

InchiKey: GPTXZZDAXLEGSA-UHFFFAOYSA-N

Formula: C21H30F2O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1

Mol. weight [g/mol]: 384.46

Physical Properties

Property code	Value	Unit	Source
gf	-635.53	kJ/mol	Joback Method
hf	-1153.75	kJ/mol	Joback Method
hfus	47.73	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.328		Crippen Method
mcvol	301.410	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	2251.00		NIST Webbook
rinpol	2251.00		NIST Webbook
tb	864.41	K	Joback Method
tc	1063.63	K	Joback Method
tf	525.81	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.84	J/mol×K	864.41	Joback Method
cpg	967.46	J/mol×K	897.61	Joback Method
cpg	981.96	J/mol×K	930.82	Joback Method
cpg	995.39	J/mol×K	964.02	Joback Method
cpg	1007.79	J/mol×K	997.22	Joback Method
cpg	1019.19	J/mol×K	1030.43	Joback Method
cpg	1029.62	J/mol×K	1063.63	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=U369327&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