Sebacic acid, heptyl 1-phenyl-2,2,2-trifluoromethylethyl ester

Inchi: InChI=1S/C25H37F3O4/c1-2-3-4-9-15-20-31-22(29)18-13-7-5-6-8-14-19-23(30)32-24(25

InchiKey: FPHQCWAHZJCNHI-UHFFFAOYSA-N

Formula: C25H37F3O4

SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 458.55

Physical Properties

Property code	Value	Unit	Source
gf	-779.84	kJ/mol	Joback Method
hf	-1414.76	kJ/mol	Joback Method
hfus	58.42	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.468		Crippen Method
mcvol	359.540	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	944.80	K	Joback Method
tc	1157.13	K	Joback Method
tf	531.44	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1203.09	J/mol×K	944.80	Joback Method
cpg	1219.97	J/mol×K	980.19	Joback Method
cpg	1235.52	J/mol×K	1015.58	Joback Method
cpg	1249.81	J/mol×K	1050.97	Joback Method
cpg	1262.92	J/mol×K	1086.36	Joback Method
cpg	1274.91	J/mol×K	1121.75	Joback Method
cpg	1285.86	J/mol×K	1157.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416805&Units=SI
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

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