Sebacic acid, dodecyl pentafluorophenyl ester

Inchi: InChI=1S/C28H41F5O4/c1-2-3-4-5-6-7-8-11-14-17-20-36-21(34)18-15-12-9-10-13-16-19
InchiKey: UBZNGALJNXLVKQ-UHFFFAOYSA-N
Formula: C28H41F5O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 536.61

Physical Properties

Property code	Value	Unit	Source
gf	-1192.75	kJ/mol	Joback Method
hf	-1912.22	kJ/mol	Joback Method
hfus	81.35	kJ/mol	Joback Method
hvap	97.73	kJ/mol	Joback Method
log10ws	-10.68		Crippen Method
logp	8.872		Crippen Method
mcvol	405.350	ml/mol	McGowan Method
pc	698.76	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook
tb	1040.55	K	Joback Method
tc	1305.98	K	Joback Method
tf	641.61	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.67	J/mol×K	1040.55	Joback Method
cpg	1418.18	J/mol×K	1084.79	Joback Method
cpg	1434.27	J/mol×K	1129.03	Joback Method
cpg	1448.01	J/mol×K	1173.27	Joback Method
cpg	1459.46	J/mol×K	1217.51	Joback Method
cpg	1468.70	J/mol×K	1261.74	Joback Method
cpg	1475.77	J/mol×K	1305.98	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=U355034&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