Sebacic acid, dodecyl pentafluorobenzyl ester

Inchi: InChI=1S/C29H43F5O4/c1-2-3-4-5-6-7-8-11-14-17-20-37-23(35)18-15-12-9-10-13-16-19
InchiKey: FQBRMHKCITWMBQ-UHFFFAOYSA-N
Formula: C29H43F5O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 550.64

Physical Properties

Property code	Value	Unit	Source
gf	-1184.33	kJ/mol	Joback Method
hf	-1932.86	kJ/mol	Joback Method
hfus	83.94	kJ/mol	Joback Method
hvap	99.96	kJ/mol	Joback Method
log10ws	-10.94		Crippen Method
logp	9.010		Crippen Method
mcvol	419.440	ml/mol	McGowan Method
pc	664.60	kPa	Joback Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1063.43	K	Joback Method
tc	1344.33	K	Joback Method
tf	652.88	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.46	J/mol×K	1063.43	Joback Method
cpg	1481.52	J/mol×K	1110.25	Joback Method
cpg	1497.86	J/mol×K	1157.06	Joback Method
cpg	1511.56	J/mol×K	1203.88	Joback Method
cpg	1522.69	J/mol×K	1250.70	Joback Method
cpg	1531.35	J/mol×K	1297.52	Joback Method
cpg	1537.61	J/mol×K	1344.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354907&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