Sebacic acid, decyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C28H41F5O5/c1-2-3-4-5-6-9-12-15-18-36-21(34)16-13-10-7-8-11-14-17-22(35

InchiKey: JIXLWAZPDVMPKO-UHFFFAOYSA-N

Formula: C28H41F5O5

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 552.61

Physical Properties

Property code	Value	Unit	Source
gf	-1297.75	kJ/mol	Joback Method
hf	-2044.44	kJ/mol	Joback Method
hfus	82.53	kJ/mol	Joback Method
hvap	100.14	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.109		Crippen Method
mcvol	411.220	ml/mol	McGowan Method
pc	692.52	kPa	Joback Method
rinpol	3034.00		NIST Webbook
rinpol	3034.00		NIST Webbook
tb	1062.97	K	Joback Method
tc	1342.62	K	Joback Method
tf	663.84	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.28	J/mol×K	1062.97	Joback Method
cpg	1444.66	J/mol×K	1109.58	Joback Method
cpg	1459.09	J/mol×K	1156.19	Joback Method
cpg	1470.61	J/mol×K	1202.79	Joback Method
cpg	1479.27	J/mol×K	1249.40	Joback Method
cpg	1485.10	J/mol×K	1296.01	Joback Method
cpg	1488.15	J/mol×K	1342.62	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=U416787&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