Sebacic acid, pentadecyl pentafluorobenzyl ester

Inchi: InChI=1S/C32H49F5O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-20-23-40-26(38)21-18-15-12-13

InchiKey: PLEBVBHDFXDRSM-UHFFFAOYSA-N

Formula: C32H49F5O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 592.72

Physical Properties

Property code	Value	Unit	Source
gf	-1159.07	kJ/mol	Joback Method
hf	-1994.78	kJ/mol	Joback Method
hfus	91.71	kJ/mol	Joback Method
hvap	106.64	kJ/mol	Joback Method
log10ws	-12.20		Crippen Method
logp	10.181		Crippen Method
mcvol	461.710	ml/mol	McGowan Method
pc	575.91	kPa	Joback Method
rinpol	3604.00		NIST Webbook
rinpol	3604.00		NIST Webbook
tb	1132.07	K	Joback Method
tc	1470.93	K	Joback Method
tf	686.69	K	Joback Method
vc	1.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.03	J/mol×K	1132.07	Joback Method
cpg	1672.76	J/mol×K	1188.55	Joback Method
cpg	1689.50	J/mol×K	1245.02	Joback Method
cpg	1702.43	J/mol×K	1301.50	Joback Method
cpg	1711.74	J/mol×K	1357.97	Joback Method
cpg	1717.60	J/mol×K	1414.45	Joback Method
cpg	1720.21	J/mol×K	1470.93	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=U354910&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