Sebacic acid, 2,2,3,3,4,4,5,5-octafluoropentyl pentyl ester

Inchi: InChI=1S/C20H30F8O4/c1-2-3-10-13-31-15(29)11-8-6-4-5-7-9-12-16(30)32-14-18(23,24)

InchiKey: DBCHCOYEEMOZPU-UHFFFAOYSA-N

Formula: C20H30F8O4

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 486.44

Physical Properties

Property code	Value	Unit	Source
gf	-1902.72	kJ/mol	Joback Method
hf	-2546.14	kJ/mol	Joback Method
hfus	52.01	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.555		Crippen Method
mcvol	321.700	ml/mol	McGowan Method
pc	895.87	kPa	Joback Method
rinpol	2159.00		NIST Webbook
rinpol	2159.00		NIST Webbook
tb	793.61	K	Joback Method
tc	971.78	K	Joback Method
tf	456.46	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.66	J/mol×K	793.61	Joback Method
cpg	1049.04	J/mol×K	823.30	Joback Method
cpg	1064.41	J/mol×K	853.00	Joback Method
cpg	1078.84	J/mol×K	882.69	Joback Method
cpg	1092.38	J/mol×K	912.39	Joback Method
cpg	1105.09	J/mol×K	942.08	Joback Method
cpg	1117.02	J/mol×K	971.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355736&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

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