Sebacic acid, octyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C26H39F3O5/c1-2-3-4-5-10-13-20-32-24(30)14-11-8-6-7-9-12-15-25(31)33-21
InchiKey: RIRWYGZAGFHGEP-UHFFFAOYSA-N
Formula: C26H39F3O5
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 488.58

Physical Properties

Property code	Value	Unit	Source
gf	-883.61	kJ/mol	Joback Method
hf	-1573.81	kJ/mol	Joback Method
hfus	65.34	kJ/mol	Joback Method
hvap	93.38	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	7.653		Crippen Method
mcvol	379.500	ml/mol	McGowan Method
pc	845.54	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	995.52	K	Joback Method
tc	1224.52	K	Joback Method
tf	592.46	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1293.29	J/mol×K	995.52	Joback Method
cpg	1310.02	J/mol×K	1033.69	Joback Method
cpg	1325.09	J/mol×K	1071.85	Joback Method
cpg	1338.57	J/mol×K	1110.02	Joback Method
cpg	1350.53	J/mol×K	1148.19	Joback Method
cpg	1361.03	J/mol×K	1186.35	Joback Method
cpg	1370.15	J/mol×K	1224.52	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=U416795&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