Sebacic acid, propyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C21H29F3O5/c1-2-15-27-19(25)9-7-5-3-4-6-8-10-20(26)28-16-17-11-13-18(14

InchiKey: NSBPWFIEOLGOQF-UHFFFAOYSA-N

Formula: C21H29F3O5

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 418.45

Physical Properties

Property code	Value	Unit	Source
gf	-925.71	kJ/mol	Joback Method
hf	-1470.61	kJ/mol	Joback Method
hfus	52.39	kJ/mol	Joback Method
hvap	82.25	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.702		Crippen Method
mcvol	309.050	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	881.12	K	Joback Method
tc	1080.15	K	Joback Method
tf	536.11	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.01	J/mol×K	881.12	Joback Method
cpg	1004.01	J/mol×K	914.29	Joback Method
cpg	1017.83	J/mol×K	947.46	Joback Method
cpg	1030.51	J/mol×K	980.64	Joback Method
cpg	1042.07	J/mol×K	1013.81	Joback Method
cpg	1052.56	J/mol×K	1046.98	Joback Method
cpg	1062.00	J/mol×K	1080.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416789&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