Sebacic acid, heptyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C24H35F3O4/c1-2-3-4-9-12-17-30-22(28)13-10-7-5-6-8-11-14-23(29)31-18-19
InchiKey: VILOYBLORRMTLA-UHFFFAOYSA-N
Formula: C24H35F3O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 444.53

Physical Properties

Property code	Value	Unit	Source
gf	-817.55	kJ/mol	Joback Method
hf	-1414.50	kJ/mol	Joback Method
hfus	65.60	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	6.782		Crippen Method
mcvol	345.450	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	2829.00		NIST Webbook
rinpol	2829.00		NIST Webbook
tb	940.53	K	Joback Method
tc	1152.88	K	Joback Method
tf	570.31	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.20	J/mol×K	940.53	Joback Method
cpg	1155.70	J/mol×K	975.92	Joback Method
cpg	1170.78	J/mol×K	1011.31	Joback Method
cpg	1184.48	J/mol×K	1046.71	Joback Method
cpg	1196.81	J/mol×K	1082.10	Joback Method
cpg	1207.82	J/mol×K	1117.49	Joback Method
cpg	1217.53	J/mol×K	1152.88	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=U380796&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