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

Inchi: InChI=1S/C21H29F3O4/c1-2-3-14-27-19(25)10-8-6-4-5-7-9-11-20(26)28-15-16-17(22)12
InchiKey: IJYKLFXKQHJZJD-UHFFFAOYSA-N
Formula: C21H29F3O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-842.81	kJ/mol	Joback Method
hf	-1352.58	kJ/mol	Joback Method
hfus	57.83	kJ/mol	Joback Method
hvap	82.46	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.611		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	871.89	K	Joback Method
tc	1068.26	K	Joback Method
tf	536.50	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.66	J/mol×K	871.89	Joback Method
cpg	973.00	J/mol×K	904.62	Joback Method
cpg	987.21	J/mol×K	937.35	Joback Method
cpg	1000.32	J/mol×K	970.08	Joback Method
cpg	1012.33	J/mol×K	1002.80	Joback Method
cpg	1023.27	J/mol×K	1035.53	Joback Method
cpg	1033.14	J/mol×K	1068.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380793&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