

Sebacic acid, butyl 1-phenyl-2,2,2-trifluoromethylethyl ester

Inchi:	InChI=1S/C22H31F3O4/c1-2-3-17-28-19(26)15-11-6-4-5-7-12-16-20(27)29-21(22(23,24)
InchiKey:	VUKBTVFAQGUROE-UHFFFAOYSA-N
Formula:	C22H31F3O4
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	416.47

Physical Properties

Property code	Value	Unit	Source
gf	-805.10	kJ/mol	Joback Method
hf	-1352.84	kJ/mol	Joback Method
hfus	50.65	kJ/mol	Joback Method
hvap	81.02	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.297		Crippen Method
mvol	317.270	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	876.16	K	Joback Method
tc	1074.69	K	Joback Method
tf	497.63	K	Joback Method
vc	1.244	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.57	J/molxK	876.16	Joback Method
cpg	1036.39	J/molxK	909.25	Joback Method
cpg	1051.07	J/molxK	942.34	Joback Method
cpg	1064.65	J/molxK	975.42	Joback Method
cpg	1077.19	J/molxK	1008.51	Joback Method
cpg	1088.74	J/molxK	1041.60	Joback Method
cpg	1099.34	J/molxK	1074.69	Joback Method

Sources

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=U416802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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