Succinic acid, pentyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C17H21F3O4/c1-2-3-4-11-23-15(21)9-10-16(22)24-12-13-5-7-14(8-6-13)17(18
InchiKey: ARERYKZCOQUFSZ-UHFFFAOYSA-N
Formula: C17H21F3O4
SMILES: CCCCCOC(=O)CCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-854.39	kJ/mol	Joback Method
hf	-1255.83	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.262		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	767.18	K	Joback Method
tc	957.59	K	Joback Method
tf	468.80	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.19	J/mol×K	767.18	Joback Method
cpg	743.32	J/mol×K	798.92	Joback Method
cpg	756.53	J/mol×K	830.65	Joback Method
cpg	768.84	J/mol×K	862.39	Joback Method
cpg	780.28	J/mol×K	894.12	Joback Method
cpg	790.87	J/mol×K	925.86	Joback Method
cpg	800.66	J/mol×K	957.59	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=U382442&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