

Sebacic acid, hexyl 4-trifluoromethoxybenzyl ester

Inchi:	InChI=1S/C24H35F3O5/c1-2-3-4-11-18-30-22(28)12-9-7-5-6-8-10-13-23(29)31-19-20-14
InchiKey:	PPIVQOUXZSTBOX-UHFFFAOYSA-N
Formula:	C24H35F3O5
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	460.53

Physical Properties

Property code	Value	Unit	Source
gf	-900.45	kJ/mol	Joback Method
hf	-1532.53	kJ/mol	Joback Method
hfus	60.16	kJ/mol	Joback Method
hvap	88.93	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	6.873		Crippen Method
mvol	351.320	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	2598.00		NIST Webbook
rinpol	2598.00		NIST Webbook
tb	949.76	K	Joback Method
tc	1163.59	K	Joback Method
tf	569.92	K	Joback Method
vc	1.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.07	J/molxK	949.76	Joback Method
cpg	1186.04	J/molxK	985.40	Joback Method
cpg	1200.58	J/molxK	1021.04	Joback Method
cpg	1213.75	J/molxK	1056.68	Joback Method
cpg	1225.59	J/molxK	1092.32	Joback Method
cpg	1236.15	J/molxK	1127.95	Joback Method
cpg	1245.49	J/molxK	1163.59	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U416793&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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