

Sebacic acid, nonyl 4-trifluoromethoxybenzyl ester

Inchi:	InChI=1S/C27H41F3O5/c1-2-3-4-5-8-11-14-21-33-25(31)15-12-9-6-7-10-13-16-26(32)34
InchiKey:	DYFDHPBBGFKKHM-UHFFFAOYSA-N
Formula:	C27H41F3O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	502.61

Physical Properties

Property code	Value	Unit	Source
gf	-875.19	kJ/mol	Joback Method
hf	-1594.45	kJ/mol	Joback Method
hfus	67.93	kJ/mol	Joback Method
hvap	95.61	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.043		Crippen Method
mvol	393.590	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	2870.00		NIST Webbook
rinpol	2870.00		NIST Webbook
tb	1018.40	K	Joback Method
tc	1256.83	K	Joback Method
tf	603.73	K	Joback Method
vc	1.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.51	J/molxK	1018.40	Joback Method
cpg	1372.67	J/molxK	1058.14	Joback Method
cpg	1388.02	J/molxK	1097.88	Joback Method
cpg	1401.65	J/molxK	1137.61	Joback Method
cpg	1413.63	J/molxK	1177.35	Joback Method
cpg	1424.06	J/molxK	1217.09	Joback Method
cpg	1433.02	J/molxK	1256.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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