

# Sebacic acid, 4-trifluoromethoxybenzyl undecyl ester

<b>Inchi:</b>	InChI=1S/C29H45F3O5/c1-2-3-4-5-6-7-10-13-16-23-35-27(33)17-14-11-8-9-12-15-18-28
<b>InchiKey:</b>	IIHANPKQLBSWLI-UHFFFAOYSA-N
<b>Formula:</b>	C29H45F3O5
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	530.66

## Physical Properties

Property code	Value	Unit	Source
gf	-858.35	kJ/mol	Joback Method
hf	-1635.73	kJ/mol	Joback Method
hfus	73.11	kJ/mol	Joback Method
hvap	100.06	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	8.823		Crippen Method
mvol	421.770	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3037.00		NIST Webbook
rinpol	3037.00		NIST Webbook
tb	1064.16	K	Joback Method
tc	1325.62	K	Joback Method
tf	626.27	K	Joback Method
vc	1.661	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.95	J/molxK	1064.16	Joback Method
cpg	1499.05	J/molxK	1107.74	Joback Method
cpg	1515.00	J/molxK	1151.31	Joback Method
cpg	1528.90	J/molxK	1194.89	Joback Method
cpg	1540.88	J/molxK	1238.47	Joback Method
cpg	1551.06	J/molxK	1282.04	Joback Method
cpg	1559.56	J/molxK	1325.62	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416798&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416798&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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