

Terephthalic acid, 4-fluorophenethyl nonyl ester

Inchi:	InChI=1S/C25H31FO4/c1-2-3-4-5-6-7-8-18-29-24(27)21-11-13-22(14-12-21)25(28)30-19
InchiKey:	CDEIDWLUZTUHGN-UHFFFAOYSA-N
Formula:	C25H31FO4
SMILES:	CCCCCCCCCOC(=O)c1ccc(C(=O)OCCc2ccc(F)cc2)cc1
Mol. weight [g/mol]:	414.51

Physical Properties

Property code	Value	Unit	Source
gf	-297.47	kJ/mol	Joback Method
hf	-794.92	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	94.61	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.133		Crippen Method
mvol	332.240	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	3155.00		NIST Webbook
rinpol	3155.00		NIST Webbook
tb	986.57	K	Joback Method
tc	1209.75	K	Joback Method
tf	594.30	K	Joback Method
vc	1.286	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1082.82	J/mol×K	986.57	Joback Method
cpg	1096.93	J/mol×K	1023.77	Joback Method
cpg	1109.61	J/mol×K	1060.96	Joback Method
cpg	1120.93	J/mol×K	1098.16	Joback Method
cpg	1130.93	J/mol×K	1135.35	Joback Method
cpg	1139.66	J/mol×K	1172.55	Joback Method
cpg	1147.18	J/mol×K	1209.75	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=U416148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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