

Fumaric acid, pentadecyl pentafluorophenyl ester

Inchi: InChI=1S/C25H33F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-33-18(31)15-16-19(32)34

InchiKey: YJRGIQAEPSJUOP-FOCLMDBBSA-N

Formula: C25H33F5O4

SMILES: CCCCCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 492.52

Physical Properties

Property code	Value	Unit	Source
gf	-1137.79	kJ/mol	Joback Method
hf	-1733.08	kJ/mol	Joback Method
hfus	73.78	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	7.478		Crippen Method
mcvol	358.780	ml/mol	McGowan Method
pc	843.58	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	976.07	K	Joback Method
tc	1202.81	K	Joback Method
tf	602.72	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1184.66	J/molxK	976.07	Joback Method
cpg	1201.00	J/molxK	1013.86	Joback Method
cpg	1215.83	J/molxK	1051.65	Joback Method
cpg	1229.19	J/molxK	1089.44	Joback Method
cpg	1241.14	J/molxK	1127.23	Joback Method
cpg	1251.71	J/molxK	1165.02	Joback Method
cpg	1260.94	J/molxK	1202.81	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=U348107&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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