

Pimelic acid, pentadecyl pentafluorobenzyl ester

Inchi:	InChI=1S/C29H43F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-37-23(35)18-15-14-16-19
InchiKey:	ROWXENHIJRBRFA-UHFFFAOYSA-N
Formula:	C29H43F5O4
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	550.64

Physical Properties

Property code	Value	Unit	Source
gf	-1184.33	kJ/mol	Joback Method
hf	-1932.86	kJ/mol	Joback Method
hfus	83.94	kJ/mol	Joback Method
hvap	99.96	kJ/mol	Joback Method
log10ws	-10.94		Crippen Method
logp	9.010		Crippen Method
mvol	419.440	ml/mol	McGowan Method
pc	664.60	kPa	Joback Method
rinpol	3294.00		NIST Webbook
rinpol	3294.00		NIST Webbook
tb	1063.43	K	Joback Method
tc	1344.33	K	Joback Method
tf	652.88	K	Joback Method
vc	1.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.46	J/molxK	1063.43	Joback Method
cpg	1481.52	J/molxK	1110.25	Joback Method
cpg	1497.86	J/molxK	1157.06	Joback Method
cpg	1511.56	J/molxK	1203.88	Joback Method
cpg	1522.69	J/molxK	1250.70	Joback Method
cpg	1531.35	J/molxK	1297.52	Joback Method
cpg	1537.61	J/molxK	1344.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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