Terephthalic acid, 2,2,3,3,3-pentafluoropropyl pentyl ester

Inchi: InChI=1S/C16H17F5O4/c1-2-3-4-9-24-13(22)11-5-7-12(8-6-11)14(23)25-10-15(17,18)16

InchiKey: SUVYUVYOFPBVJJ-UHFFFAOYSA-N

Formula: C16H17F5O4

SMILES: CCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 368.30

Physical Properties

Property code	Value	Unit	Source
gf	-1249.59	kJ/mol	Joback Method
hf	-1636.16	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	65.78	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.388		Crippen Method
mcvol	236.270	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	739.61	K	Joback Method
tc	925.84	K	Joback Method
tf	461.13	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.63	J/mol×K	739.61	Joback Method
cpg	704.70	J/mol×K	770.65	Joback Method
cpg	716.89	J/mol×K	801.69	Joback Method
cpg	728.24	J/mol×K	832.73	Joback Method
cpg	738.78	J/mol×K	863.77	Joback Method
cpg	748.56	J/mol×K	894.80	Joback Method
cpg	757.61	J/mol×K	925.84	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=U415776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/122-036-6/Terephthalic-acid-2-2-3-3-3-pentafluoropropyl-pentyl-ester.pdf
Generated by Cheméo on 2024-05-10 20:52:22.00583212 +0000 UTC m=+17663590.926409436.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.