Terephthalic acid, 2,2,3,4,4,4-hexafluorobutyl octyl ester

Inchi: InChI=1S/C20H24F6O4/c1-2-3-4-5-6-7-12-29-16(27)14-8-10-15(11-9-14)17(28)30-13-19

InchiKey: MYXUSVMHEUVFCE-UHFFFAOYSA-N

Formula: C20H24F6O4

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

Mol. weight [g/mol]: 442.39

Physical Properties

Property code	Value	Unit	Source
gf	-1413.16	kJ/mol	Joback Method
hf	-1920.11	kJ/mol	Joback Method
hfus	46.91	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.896		Crippen Method
mcvol	294.400	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	2421.00		NIST Webbook
tb	829.96	K	Joback Method
tc	1019.20	K	Joback Method
tf	491.80	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.85	J/mol×K	829.96	Joback Method
cpg	939.08	J/mol×K	861.50	Joback Method
cpg	952.32	J/mol×K	893.04	Joback Method
cpg	964.62	J/mol×K	924.58	Joback Method
cpg	976.03	J/mol×K	956.12	Joback Method
cpg	986.60	J/mol×K	987.66	Joback Method
cpg	996.38	J/mol×K	1019.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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