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

Inchi: InChI=1S/C20H23F7O4/c1-2-3-4-5-6-7-12-30-16(28)14-8-10-15(11-9-14)17(29)31-13-18

InchiKey: AFXMXCQCIYWYEH-UHFFFAOYSA-N

Formula: C20H23F7O4

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

Mol. weight [g/mol]: 460.38

Physical Properties

Property code	Value	Unit	Source
gf	-1602.69	kJ/mol	Joback Method
hf	-2119.69	kJ/mol	Joback Method
hfus	46.10	kJ/mol	Joback Method
hvap	71.76	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.194		Crippen Method
mcvol	296.170	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	826.44	K	Joback Method
tc	1014.70	K	Joback Method
tf	509.81	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.01	J/mol×K	826.44	Joback Method
cpg	946.85	J/mol×K	857.82	Joback Method
cpg	959.73	J/mol×K	889.19	Joback Method
cpg	971.72	J/mol×K	920.57	Joback Method
cpg	982.88	J/mol×K	951.95	Joback Method
cpg	993.28	J/mol×K	983.33	Joback Method
cpg	1002.98	J/mol×K	1014.70	Joback Method

Sources

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=U415942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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