2-[2-[2-[2-[2-[2-(2,2,3,3,4,4,4-Heptafluorobutanoyl)
2,2,3,3,4,4,4-heptafluorobutanoate

Other names: 20,20,21,21,22,22,22-Heptafluoro-19-oxo-3,6,9,12,15,18-hexaoxadocos-1-yl heptafluorobutyrate; Hexaethylene glycol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C20H24F14O9/c21-15(22,17(25,26)19(29,30)31)13(35)42-11-9-40-7-5-38-3-1-

InchiKey: DWSNSRVFOZDBFX-UHFFFAOYSA-N

Formula: C20H24F14O9

SMILES: O=C(OCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F

Mol. weight [g/mol]: 674.38

Physical Properties

Property code	Value	Unit	Source
gf	-3585.62	kJ/mol	Joback Method
hf	-4404.87	kJ/mol	Joback Method
hfus	57.71	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.822		Crippen Method
mcvol	361.670	ml/mol	McGowan Method
pc	751.85	kPa	Joback Method
rinpol	1988.90		NIST Webbook
tb	892.08	K	Joback Method
tc	1116.52	K	Joback Method
tf	593.41	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.75	J/mol×K	892.08	Joback Method
cpg	1242.01	J/mol×K	929.49	Joback Method
cpg	1255.66	J/mol×K	966.89	Joback Method
cpg	1267.80	J/mol×K	1004.30	Joback Method
cpg	1278.55	J/mol×K	1041.71	Joback Method
cpg	1287.99	J/mol×K	1079.11	Joback Method
cpg	1296.24	J/mol×K	1116.52	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=U352028&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

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