2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2,2,3,3,4,4,4-Heptafluorobu
2,2,3,3,4,4,4-heptafluorobutanoate

Othernames: 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80,83,86,89,92,95,98,101,104,107,110,113,116,119,122,125,128,131,134,137,140,143,146,149,152,155,158,161,164,167,170,173,176,179,182,185,188,191,194,197,200,203,206,209,212,215,218,221,224,227-nonaoxahentriacont-1-yl heptafluorobutyrate; Nonaethylene glycol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C26H36F14O12/c27-21(28,23(31,32)25(35,36)37)19(41)51-17-15-49-13-11-47

InchiKey: BRWSJVORUVRDIK-UHFFFAOYSA-N

Formula: C26H36F14O12

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

Mol. weight [g/mol]: 806.53

Physical Properties

Property code	Value	Unit	Source
gf	-3850.10	kJ/mol	Joback Method
hf	-4925.37	kJ/mol	Joback Method
hfus	76.81	kJ/mol	Joback Method
hvap	91.85	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.871		Crippen Method
mcvol	463.820	ml/mol	McGowan Method
pc	547.43	kPa	Joback Method
rinpol	2685.50		NIST Webbook
tb	1096.62	K	Joback Method
tc	1505.48	K	Joback Method
tf	727.72	K	Joback Method
vc	1.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1665.49	J/mol×K	1096.62	Joback Method
cpg	1681.41	J/mol×K	1164.76	Joback Method
cpg	1691.23	J/mol×K	1232.91	Joback Method
cpg	1695.39	J/mol×K	1301.05	Joback Method
cpg	1694.35	J/mol×K	1369.19	Joback Method
cpg	1688.58	J/mol×K	1437.34	Joback Method
cpg	1678.53	J/mol×K	1505.48	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=U352025&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