Heneicosyl heptafluorobutyrate

Other names:	Heneicosyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Heneicosanol, heptafluorobutyrate
	Heneicosyl perfluorobutyrate
Inchi:	InChI=1S/C25H43F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-34-22
InchiKey:	RFTHPDMPTLHVMV-UHFFFAOYSA-N
Formula:	C25H43F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	508.60

Physical Properties

Property code	Value	Unit	Source
gf	-1429.45	kJ/mol	Joback Method
hf	-2203.15	kJ/mol	Joback Method
hfus	62.61	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	9.794		Crippen Method
mcvol	382.940	ml/mol	McGowan Method
pc	681.71	kPa	Joback Method
rinpol	2318.60		NIST Webbook
tb	832.89	K	Joback Method
tc	1024.54	K	Joback Method
tf	455.06	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.39	J/mol×K	832.89	Joback Method
cpg	1293.51	J/mol×K	864.83	Joback Method
cpg	1313.42	J/mol×K	896.77	Joback Method
cpg	1332.20	J/mol×K	928.72	Joback Method
cpg	1349.95	J/mol×K	960.66	Joback Method
cpg	1366.75	J/mol×K	992.60	Joback Method

cpg	1382.71	J/mol×K	1024.54	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=U351838&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