Heptafluorobutyric acid, n-octadecyl ester

Other names:	Octadecyl heptafluorobutyrate
	Octadecyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Octadecanol, heptafluorobutyrate
	Octadecyl perfluorobutyrate
	Octadecyl heptafluorobutanoate
	Heptafluorobutyric acid, octadecyl ester
Inchi:	InChI=1S/C22H37F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-31-19(30)20(23
InchiKey:	ABJHYFXBHBSPMK-UHFFFAOYSA-N
Formula:	C22H37F7O2
SMILES:	CCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	466.52
CAS:	400-57-7

Physical Properties

Property code	Value	Unit	Source
gf	-1454.71	kJ/mol	Joback Method
hf	-2141.23	kJ/mol	Joback Method
hfus	54.84	kJ/mol	Joback Method
hvap	64.12	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	8.624		Crippen Method
mcvol	340.670	ml/mol	McGowan Method
pc	797.08	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2037.70		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2037.70		NIST Webbook
ripol	2095.00		NIST Webbook
tb	764.25	K	Joback Method
tc	935.69	K	Joback Method
tf	421.25	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.72	J/mol×K	764.25	Joback Method
cpg	1105.58	J/mol×K	792.82	Joback Method
cpg	1123.42	J/mol×K	821.40	Joback Method
cpg	1140.31	J/mol×K	849.97	Joback Method
cpg	1156.30	J/mol×K	878.54	Joback Method
cpg	1171.46	J/mol×K	907.12	Joback Method
cpg	1185.85	J/mol×K	935.69	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C400577&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume