Butyl perfluoroheptanoate

Other names: 2,2,3,3,4,4,5,5,6,6,7,7,7-Tridecafluoro-heptanoic acid butyl ester
Inchi: InChI=1S/C11H9F13O2/c1-2-3-4-26-5(25)6(12,13)7(14,15)8(16,17)9(18,19)10(20,21)11(
InchiKey: GXVAUAFNGNFJBL-UHFFFAOYSA-N
Formula: C11H9F13O2
SMILES: CCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 420.17

Physical Properties

Property code	Value	Unit	Source
gf	-2707.67	kJ/mol	Joback Method
hf	-3117.10	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	30.84	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.069		Crippen Method
mcvol	196.300	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	898.00		NIST Webbook
rinpol	898.40		NIST Webbook
tb	498.50	K	Joback Method
tc	633.35	K	Joback Method
tf	308.08	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.89	J/mol×K	498.50	Joback Method
cpg	550.94	J/mol×K	520.98	Joback Method
cpg	563.17	J/mol×K	543.45	Joback Method
cpg	574.61	J/mol×K	565.93	Joback Method
cpg	585.31	J/mol×K	588.40	Joback Method
cpg	595.30	J/mol×K	610.88	Joback Method
cpg	604.63	J/mol×K	633.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70044&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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