Sarcosine, N-heptafluorobutyryl-, ethyl ester

Inchi: InChI=1S/C9H10F7NO3/c1-3-20-5(18)4-17(2)6(19)7(10,11)8(12,13)9(14,15)16/h3-4H2,1
InchiKey: RUOVTXQTJMRODG-UHFFFAOYSA-N
Formula: C9H10F7NO3
SMILES: CCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 313.17

Physical Properties

Property code	Value	Unit	Source
hf	-2051.29	kJ/mol	Cheméo Relay (1.0)
hfus	25.79	kJ/mol	Joback Method
hvap	63.92	kJ/mol	Cheméo Relay (1.0)
logp	1.841		Crippen Method
mcvol	169.050	ml/mol	McGowan Method
rinpol	980.00		NIST Webbook
tb	453.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.51	J/mol×K	533.12	Joback Method
cpg	457.18	J/mol×K	559.19	Joback Method
cpg	468.13	J/mol×K	585.27	Joback Method
cpg	478.39	J/mol×K	611.34	Joback Method
cpg	488.00	J/mol×K	637.42	Joback Method
cpg	496.99	J/mol×K	663.49	Joback Method
cpg	505.38	J/mol×K	689.56	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321254&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature