

TEA
Inchikey:

SDWGRHDRWRURPJ-UHFFFAOYSA-N

Formula:

C21H39F3O7

SMILES:

CCCCCCCCCOCOCOCOCOCOC(=O)C(F)(F)F

Mol. weight [g/mol]:

460.53

Physical Properties

Property code	Value	Unit	Source
gf	-1214.57	kJ/mol	Joback Method
hf	-1979.75	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.925		Crippen Method
mcvol	348.850	ml/mol	McGowan Method
pc	870.68	kPa	Joback Method
rinpol	2497.00		NIST Webbook
tb	862.85	K	Joback Method
tc	1059.69	K	Joback Method
tf	513.93	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.09	J/mol×K	862.85	Joback Method
cpg	1175.02	J/mol×K	895.66	Joback Method
cpg	1192.48	J/mol×K	928.46	Joback Method
cpg	1208.46	J/mol×K	961.27	Joback Method
cpg	1222.98	J/mol×K	994.08	Joback Method
cpg	1236.01	J/mol×K	1026.89	Joback Method
cpg	1247.57	J/mol×K	1059.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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=R184184&Units=SI

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
hvac:	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

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