

Pentafluoropropionic acid, dodecyl ester

Other names:

Dodecyl pentafluoropropionate
Dodecyl 2,2,3,3,3-pentafluoropropanoate
1-Dodecanol, pentafluoropropionate
1-Dodecanol, PFP

Inchi:

InChI=1S/C15H25F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-22-13(21)14(16,17)15(18,19)20/h2

InchiKey:

XIQJAGXFOCELKQ-UHFFFAOYSA-N

Formula:

C15H25F5O2

SMILES:

CCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]:

332.35

CAS:

6222-04-4

Physical Properties

Property code	Value	Unit	Source
gf	-1126.87	kJ/mol	Joback Method
hf	-1595.78	kJ/mol	Joback Method
hfus	37.96	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.648		Crippen Method
mcvol	238.500	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	1442.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1455.60		NIST Webbook
ripol	1505.00		NIST Webbook
tb	608.78	K	Joback Method
tc	762.79	K	Joback Method
tf	338.76	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.86	J/molxK	608.78	Joback Method

cpg	681.64	J/mol×K	634.45	Joback Method
cpg	696.67	J/mol×K	660.12	Joback Method
cpg	710.99	J/mol×K	685.79	Joback Method
cpg	724.62	J/mol×K	711.46	Joback Method
cpg	737.59	J/mol×K	737.13	Joback Method
cpg	749.93	J/mol×K	762.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6222044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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