

1-Dodecanol, heptafluorobutyrate

Other names:	Heptafluorobutyric acid, dodecyl ester Dodecyl heptafluorobutanoate
Inchi:	InChI=1S/C16H25F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-25-13(24)14(17,18)15(19,20)16(21)
InchiKey:	VHUDBNCZZWHQHU-UHFFFAOYSA-N
Formula:	C16H25F7O2
SMILES:	CCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	382.36
CAS:	6222-08-8

Physical Properties

Property code	Value	Unit	Source
gf	-1505.23	kJ/mol	Joback Method
hf	-2017.39	kJ/mol	Joback Method
hfus	39.30	kJ/mol	Joback Method
hvap	50.76	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	6.283		Crippen Method
mcvol	256.130	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	1486.30		NIST Webbook
rinpol	1486.30		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1505.00		NIST Webbook
tb	626.97	K	Joback Method
tc	778.69	K	Joback Method
tf	353.63	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.76	J/mol×K	626.97	Joback Method
cpg	754.53	J/mol×K	652.26	Joback Method
cpg	769.51	J/mol×K	677.54	Joback Method
cpg	783.73	J/mol×K	702.83	Joback Method
cpg	797.22	J/mol×K	728.11	Joback Method
cpg	810.03	J/mol×K	753.40	Joback Method
cpg	822.18	J/mol×K	778.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6222088&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
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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