

Dotriacontyl heptafluorobutyrate

Other names:	Dotriacontyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Dotriacontanol, heptafluorobutyrate Dotriacontyl perfluorobutyrate
Inchi:	InChI=1S/C36H65F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	HDYLMIWYXVQKDS-UHFFFAOYSA-N
Formula:	C36H65F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	662.89

Physical Properties

Property code	Value	Unit	Source
gf	-1336.83	kJ/mol	Joback Method
hf	-2430.19	kJ/mol	Joback Method
hfus	91.10	kJ/mol	Joback Method
hvap	95.28	kJ/mol	Joback Method
log10ws	-15.04		Crippen Method
logp	14.085		Crippen Method
mcvol	537.930	ml/mol	McGowan Method
pc	418.88	kPa	Joback Method
rinpol	3370.90		NIST Webbook
tb	1084.57	K	Joback Method
tc	1458.04	K	Joback Method
tf	579.03	K	Joback Method
vc	2.168	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1997.21	J/mol×K	1084.57	Joback Method
cpg	2036.49	J/mol×K	1146.82	Joback Method
cpg	2073.11	J/mol×K	1209.06	Joback Method
cpg	2107.96	J/mol×K	1271.31	Joback Method
cpg	2141.92	J/mol×K	1333.55	Joback Method
cpg	2175.87	J/mol×K	1395.80	Joback Method

Sources

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=U351842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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