

Tetratriacontyl heptafluorobutyrate

Other names:	Tetratriacontyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Tetratriacontanol, heptafluorobutyrate Tetratriacontyl perfluorobutyrate
Inchi:	InChI=1S/C38H69F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	DGGUHEYSIUTPKS-UHFFFAOYSA-N
Formula:	C38H69F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	690.94

Physical Properties

Property code	Value	Unit	Source
gf	-1319.99	kJ/mol	Joback Method
hf	-2471.47	kJ/mol	Joback Method
hfus	96.28	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-15.88		Crippen Method
logp	14.866		Crippen Method
mcvol	566.110	ml/mol	McGowan Method
pc	387.81	kPa	Joback Method
rinpol	3567.20		NIST Webbook
rinpol	3567.20		NIST Webbook
tb	1130.33	K	Joback Method
tc	1565.55	K	Joback Method
tf	601.57	K	Joback Method
vc	2.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2134.69	J/mol×K	1130.33	Joback Method
cpg	2180.29	J/mol×K	1202.87	Joback Method
cpg	2223.12	J/mol×K	1275.40	Joback Method
cpg	2264.63	J/mol×K	1347.94	Joback Method
cpg	2306.27	J/mol×K	1420.47	Joback Method

cpg	2349.48	J/mol×K	1493.01	Joback Method
cpg	2395.71	J/mol×K	1565.55	Joback Method

Sources

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=U351841&Units=SI
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
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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