

Tetracosyl heptafluorobutyrate

Other names:	Tetracosyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Tetracosanol, heptafluorobutyrate Tetracosyl perfluorobutyrate
Inchi:	InChI=1S/C28H49F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	CCOUVFHNEXWUAW-UHFFFAOYSA-N
Formula:	C28H49F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	550.68

Physical Properties

Property code	Value	Unit	Source
gf	-1404.19	kJ/mol	Joback Method
hf	-2265.07	kJ/mol	Joback Method
hfus	70.38	kJ/mol	Joback Method
hvap	77.47	kJ/mol	Joback Method
log10ws	-11.70		Crippen Method
logp	10.965		Crippen Method
mcvol	425.210	ml/mol	McGowan Method
pc	589.69	kPa	Joback Method
rinpol	2602.30		NIST Webbook
rinpol	2602.30		NIST Webbook
tb	901.53	K	Joback Method
tc	1123.17	K	Joback Method
tf	488.87	K	Joback Method
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1464.01	J/mol×K	901.53	Joback Method
cpg	1488.23	J/mol×K	938.47	Joback Method
cpg	1510.94	J/mol×K	975.41	Joback Method
cpg	1532.29	J/mol×K	1012.35	Joback Method
cpg	1552.43	J/mol×K	1049.29	Joback Method

cpg	1571.52	J/mol×K	1086.23	Joback Method
cpg	1589.71	J/mol×K	1123.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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