

Tricosyl heptafluorobutyrate

Other names:	Tricosyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Tricosanol, heptafluorobutyrate Tricosyl perfluorobutyrate
Inchi:	InChI=1S/C27H47F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	QBPVDTZBRPTPJO-UHFFFAOYSA-N
Formula:	C27H47F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	536.65

Physical Properties

Property code	Value	Unit	Source
gf	-1412.61	kJ/mol	Joback Method
hf	-2244.43	kJ/mol	Joback Method
hfus	67.79	kJ/mol	Joback Method
hvap	75.25	kJ/mol	Joback Method
log10ws	-11.28		Crippen Method
logp	10.575		Crippen Method
mcvol	411.120	ml/mol	McGowan Method
pc	618.18	kPa	Joback Method
rinpol	2506.90		NIST Webbook
rinpol	2506.90		NIST Webbook
tb	878.65	K	Joback Method
tc	1089.05	K	Joback Method
tf	477.60	K	Joback Method
vc	1.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1399.54	J/molxK	878.65	Joback Method
cpg	1422.62	J/molxK	913.72	Joback Method
cpg	1444.30	J/molxK	948.78	Joback Method
cpg	1464.70	J/molxK	983.85	Joback Method
cpg	1483.95	J/molxK	1018.91	Joback Method

cpg	1502.19	J/mol×K	1053.98	Joback Method
cpg	1519.54	J/mol×K	1089.05	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=U351834&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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