

Tricosyl pentafluoropropionate

Other names:	Tricosyl 2,2,3,3,3-pentafluoropropanoate 1-Tricosanol, pentafluoropropionate
Inchi:	InChI=1S/C26H47F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	WJBCEVFPSUTMSD-UHFFFAOYSA-N
Formula:	C26H47F5O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	486.64

Physical Properties

Property code	Value	Unit	Source
gf	-1034.25	kJ/mol	Joback Method
hf	-1822.82	kJ/mol	Joback Method
hfus	66.45	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-10.54		Crippen Method
logp	9.939		Crippen Method
mcvol	393.490	ml/mol	McGowan Method
pc	672.90	kPa	Joback Method
rinpol	2482.70		NIST Webbook
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tb	860.46	K	Joback Method
tc	1060.00	K	Joback Method
tf	462.73	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.12	J/molxK	860.46	Joback Method
cpg	1343.47	J/molxK	893.72	Joback Method
cpg	1364.51	J/molxK	926.97	Joback Method
cpg	1384.31	J/molxK	960.23	Joback Method
cpg	1402.98	J/molxK	993.49	Joback Method
cpg	1420.58	J/molxK	1026.75	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=U351810&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
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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