Docosyl pentafluoropropionate

Other names: Docosyl 2,2,3,3,3-pentafluoropropanoate
1-Docosanol, pentafluoropropionate
Inchi: InChI=1S/C25H45F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-32
InchiKey: KEKXEGYQJNXSCS-UHFFFAOYSA-N
Formula: C25H45F5O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 472.62

Physical Properties

Property code	Value	Unit	Source
gf	-1042.67	kJ/mol	Joback Method
hf	-1802.18	kJ/mol	Joback Method
hfus	63.87	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-10.13		Crippen Method
logp	9.549		Crippen Method
mcvol	379.400	ml/mol	McGowan Method
pc	707.71	kPa	Joback Method
rinpol	2384.10		NIST Webbook
tb	837.58	K	Joback Method
tc	1028.87	K	Joback Method
tf	451.46	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.43	J/mol×K	837.58	Joback Method
cpg	1278.91	J/mol×K	869.46	Joback Method
cpg	1299.17	J/mol×K	901.34	Joback Method
cpg	1318.28	J/mol×K	933.22	Joback Method
cpg	1336.31	J/mol×K	965.10	Joback Method
cpg	1353.35	J/mol×K	996.98	Joback Method
cpg	1369.46	J/mol×K	1028.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351809&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