

trans-2-Dodecen-1-ol, pentafluoropropionate

Inchi:	InChI=1S/C15H23F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-22-13(21)14(16,17)15(18,19)20/h1
InchiKey:	XQULQGQTCWDDGX-ZHACJKMWSA-N
Formula:	C15H23F5O2
SMILES:	CCCCCCCCC=CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	330.33

Physical Properties

Property code	Value	Unit	Source
gf	-1046.65	kJ/mol	Joback Method
hf	-1478.56	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.424		Crippen Method
mvol	234.200	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	1443.10		NIST Webbook
rinpol	1443.10		NIST Webbook
tb	612.94	K	Joback Method
tc	771.32	K	Joback Method
tf	333.68	K	Joback Method
vc	0.948	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.98	J/mol×K	612.94	Joback Method
cpg	661.30	J/mol×K	639.34	Joback Method
cpg	675.84	J/mol×K	665.73	Joback Method
cpg	689.65	J/mol×K	692.13	Joback Method
cpg	702.76	J/mol×K	718.53	Joback Method
cpg	715.21	J/mol×K	744.92	Joback Method
cpg	727.03	J/mol×K	771.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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