trans-2-Dodecen-1-ol, heptafluorobutyrate

Inchi: InChI=1S/C16H23F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-25-13(24)14(17,18)15(19,20)16(21
InchiKey: KZMYZWHQTQVIND-ZHACJKMWSA-N
Formula: C16H23F7O2
SMILES: CCCCCCCCCC=CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 380.34

Physical Properties

Property code	Value	Unit	Source
gf	-1425.01	kJ/mol	Joback Method
hf	-1900.17	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	50.72	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.059		Crippen Method
mcvol	251.830	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	1481.20		NIST Webbook
tb	631.13	K	Joback Method
tc	786.52	K	Joback Method
tf	348.55	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.39	J/mol×K	631.13	Joback Method
cpg	733.65	J/mol×K	657.03	Joback Method
cpg	748.09	J/mol×K	682.93	Joback Method
cpg	761.77	J/mol×K	708.83	Joback Method
cpg	774.71	J/mol×K	734.73	Joback Method
cpg	786.97	J/mol×K	760.62	Joback Method
cpg	798.59	J/mol×K	786.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352260&Units=SI

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