Decyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C15H28O2/c1-4-6-7-8-9-10-11-12-13-17-15(16)14(3)5-2/h5H,4,6-13H2,1-3H3/
InchiKey: UCGAWLWEQSSTNO-LHHJGKSTSA-N
Formula: C15H28O2
SMILES: CC=C(C)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-86.83	kJ/mol	Joback Method
hf	-490.30	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	622.93	K	Joback Method
tc	798.18	K	Joback Method
tf	311.93	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.32	J/mol×K	622.93	Joback Method
cpg	617.53	J/mol×K	652.14	Joback Method
cpg	633.97	J/mol×K	681.35	Joback Method
cpg	649.67	J/mol×K	710.55	Joback Method
cpg	664.64	J/mol×K	739.76	Joback Method
cpg	678.92	J/mol×K	768.97	Joback Method
cpg	692.52	J/mol×K	798.18	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=U373711&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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