Docosyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C27H52O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: ZBTJCBFSOLLYFO-MBAGFTIUSA-N
Formula: C27H52O2
SMILES: CC=C(C)C(=O)OCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 408.70

Physical Properties

Property code	Value	Unit	Source
gf	14.21	kJ/mol	Joback Method
hf	-737.98	kJ/mol	Joback Method
hfus	67.37	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-9.84		Crippen Method
logp	9.318		Crippen Method
mcvol	394.430	ml/mol	McGowan Method
pc	727.70	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	897.49	K	Joback Method
tc	1100.54	K	Joback Method
tf	447.17	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1323.65	J/mol×K	897.49	Joback Method
cpg	1346.52	J/mol×K	931.33	Joback Method
cpg	1368.07	J/mol×K	965.17	Joback Method
cpg	1388.38	J/mol×K	999.01	Joback Method
cpg	1407.50	J/mol×K	1032.85	Joback Method
cpg	1425.51	J/mol×K	1066.69	Joback Method
cpg	1442.47	J/mol×K	1100.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373751&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